EE2211 Lecture 7: Overfitting, Model Complexity, Feature Selection & Regularization, Bias-Variance Tradeoff

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Acknowledgements to

Xinchao, Helen, Thomas, Kar Ann, Chen Khong, Robby, and Haizhou

Outline

1 Review of Regression

Review of Regression

- Goal: Given feature(s) $\mathbf{x} \in \mathbb{R}^d$, we want to predict target $y \in \mathbb{R}$.
  1. $\mathbf{x}$ can be one-dimensional (in which case we may write x);
  2. Or $\mathbf{x}$ may be high dimensional;
  3. y is often one-dimensional (trying to predict one output).

- Two types of input data
  1. Training Set $\{(\mathbf{x}_i, y_i)\}_{i=1}^m$;
  2. Test Set $\{\mathbf{x}_j\}_{j=m+1}^n$ (no targets) [We called one of these samples $\mathbf{x}_{\text{new}}$ previously];

- m training samples, n test samples, all in $\mathbb{R}^d$

- Learning/Training
  Training set used to estimate regression coefficients $\bar{\mathbf{w}}^*$.

- Testing/Prediction
  Prediction performed on test set to evaluate performance.

Review of Regression: Linear Case

- Suppose the feature is one-dimensional $x \in \mathbb{R}$.
- Want to learn the affine relationship between x and $y \in \mathbb{R}$.
- With $m = 4$ training samples, the design matrix and target vector are

$$\mathbf{X} = \begin{bmatrix} 1 & x_1 \\ 1 & x_2 \\ 1 & x_3 \\ 1 & x_4 \end{bmatrix} \quad \text{and} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}$$

- Learning/Training

$$\bar{\mathbf{w}}^* = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y}.$$

- Testing/Prediction on x_{new}

$$y_{\text{test}} = \begin{bmatrix} 1 \\ x_{\text{new}} \end{bmatrix}^\top \bar{\mathbf{w}}^*.$$

Regression Review: Polynomial

- Features $\mathbf{x} \in \mathbb{R}^d$ may be one-dimensional or high dimensional; $y \in \mathbb{R}$ is a one-dimensional target as usual.
- Want to learn a polynomial relationship between x and y
- Quadratic illustration ($m = 4$ training samples and x is one-dim) of design matrix and target vector

$$\mathbf{X} = \begin{bmatrix} 1 & x_1 & x_1^2 \\ 1 & x_2 & x_2^2 \\ 1 & x_3 & x_3^2 \\ 1 & x_4 & x_4^2 \end{bmatrix} \quad \text{and} \quad \mathbf{y} = \begin{bmatrix} y_1 \\ y_2 \\ y_3 \\ y_4 \end{bmatrix}$$

- Learning/Training

$$\bar{\mathbf{w}}^* = (\mathbf{X}^\top \mathbf{X})^{-1} \mathbf{X}^\top \mathbf{y} \in \mathbb{R}^3.$$

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$$y_{\text{test}} = \begin{bmatrix} 1 \\ x_{\text{new}} \\ x_{\text{new}}^2 \end{bmatrix}^\top \bar{\mathbf{w}}^*.$$

Polynomial Regression Review: Notation

- Sometimes, we use the notation $\mathbf{P}$ in place of $\mathbf{X}$ to emphasize that the features $\mathbf{x}$ are encoded in a polynomial way in the design matrix $\mathbf{P} = \mathbf{X}$.
- Learning/Training

$$\bar{\mathbf{w}}^* = (\mathbf{P}^\top \mathbf{P})^{-1} \mathbf{P}^\top \mathbf{y} \in \mathbb{R}^3.$$

- Testing/Prediction on x_{new}

$$y_{\mathrm{new}} = \underbrace{\begin{bmatrix} 1 \\ x_{\mathrm{new}} \\ \color{red}{x_{\mathrm{new}}^2} \end{bmatrix}^\top}_{= \mathbf{p}_{\mathrm{new}}^\top} \bar{\mathbf{w}}^*.$$

Note on Training & Test Sets

- Affine is special case of polynomial
- Use $\mathbf{P}$ instead of $\mathbf{X}$ from now on.
- Training/Learning (primal) on training set

$$\bar{\mathbf{w}}^* = (\mathbf{P}^\top \mathbf{P})^{-1} \mathbf{P}^\top \mathbf{y} \in \mathbb{R}^{d'}.$$

- Prediction/Testing on the entire test set

$$\mathbf{y}_{\mathrm{new}} = \mathbf{P}_{\mathrm{new}} \bar{\mathbf{w}}^* \in \mathbb{R}^n$$

where

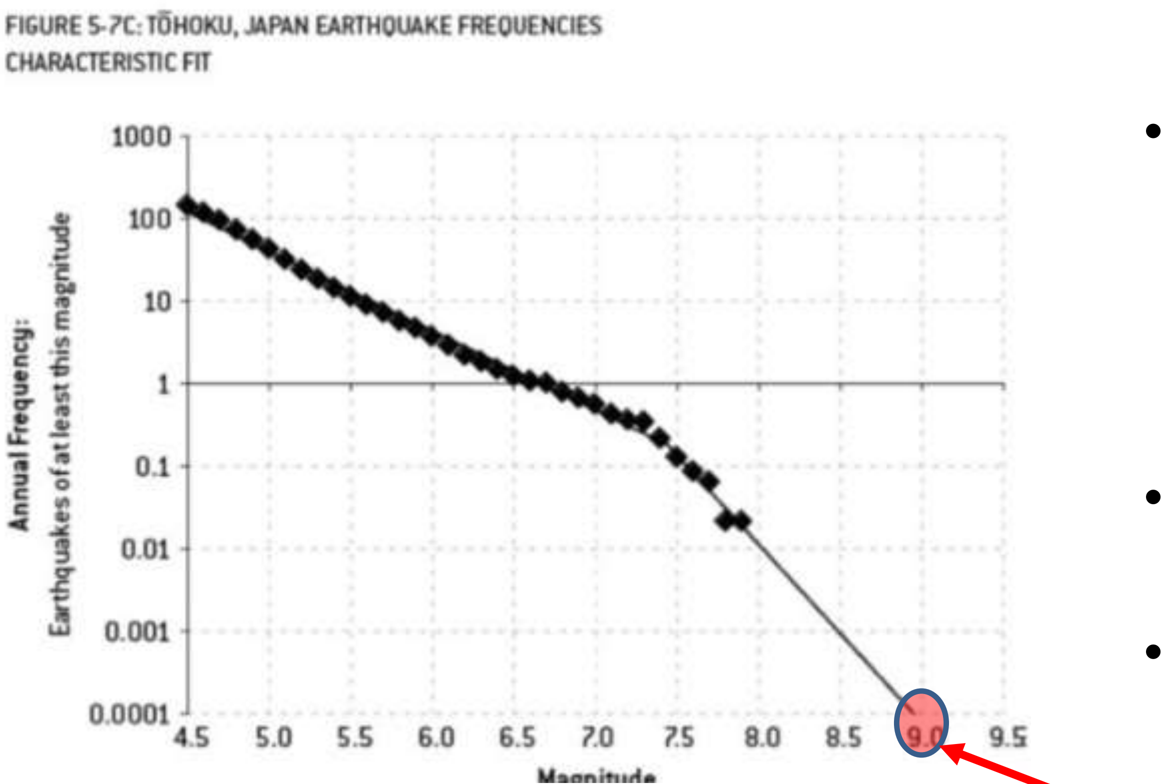
$$\mathbf{P}_{\mathrm{new}} = \begin{bmatrix} \mathbf{p}_{m+1}^\top \\ \mathbf{p}_{m+2}^\top \\ \vdots \\ \mathbf{p}_{m+n}^\top \end{bmatrix} \in \mathbb{R}^{n \times d'}$$

Note on Training & Test Sets

- There should be zero overlap between training & test sets.
- Important goal of regression: prediction on new unseen data, i.e., the test set.
- Question: Why is test set important for evaluation?

Questions?

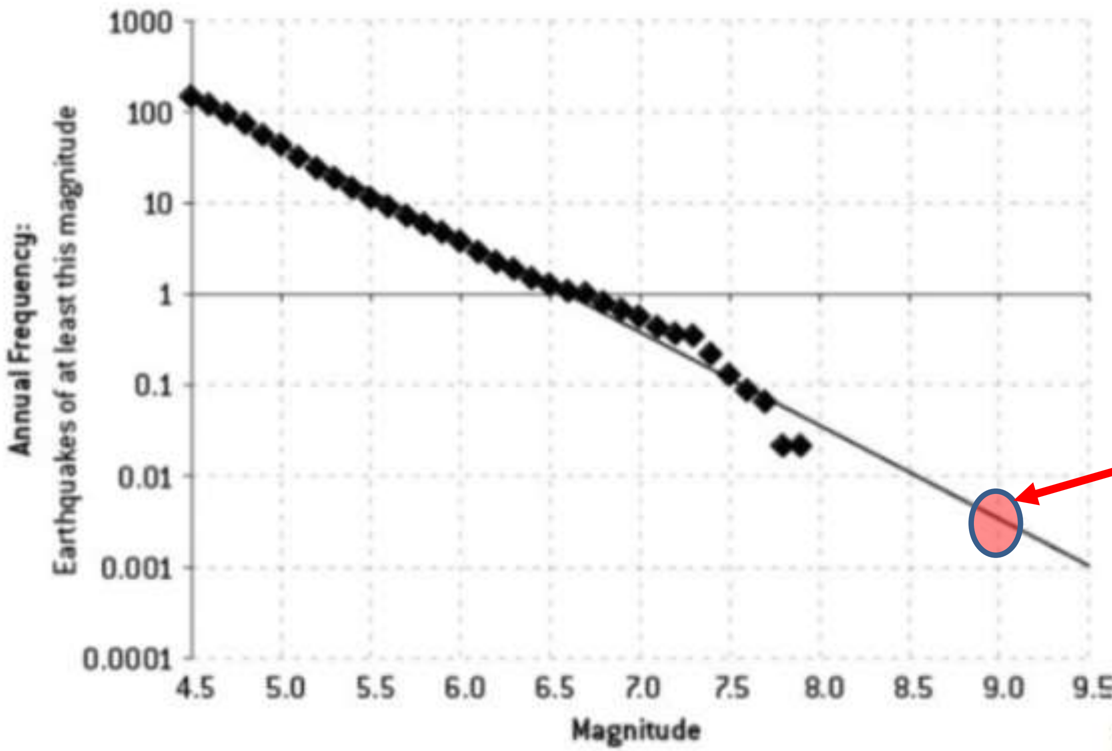
Overfitting Motivation: Fukushima Disaster



- In March 2011, there was a large earthquake in Japan.
- Small earthquakes occur frequently while massive earthquakes occur rarely.
- Engineers fitted a polynomial model
- Earthquake of magnitude 9.0 occurs once every 10,000 years

Overfitting Motivation: Fukushima Disaster

FIGURE 5-7B: TŌHOKU, JAPAN EARTHQUAKE FREQUENCIES
GUTENBERG-RICHTER FIT



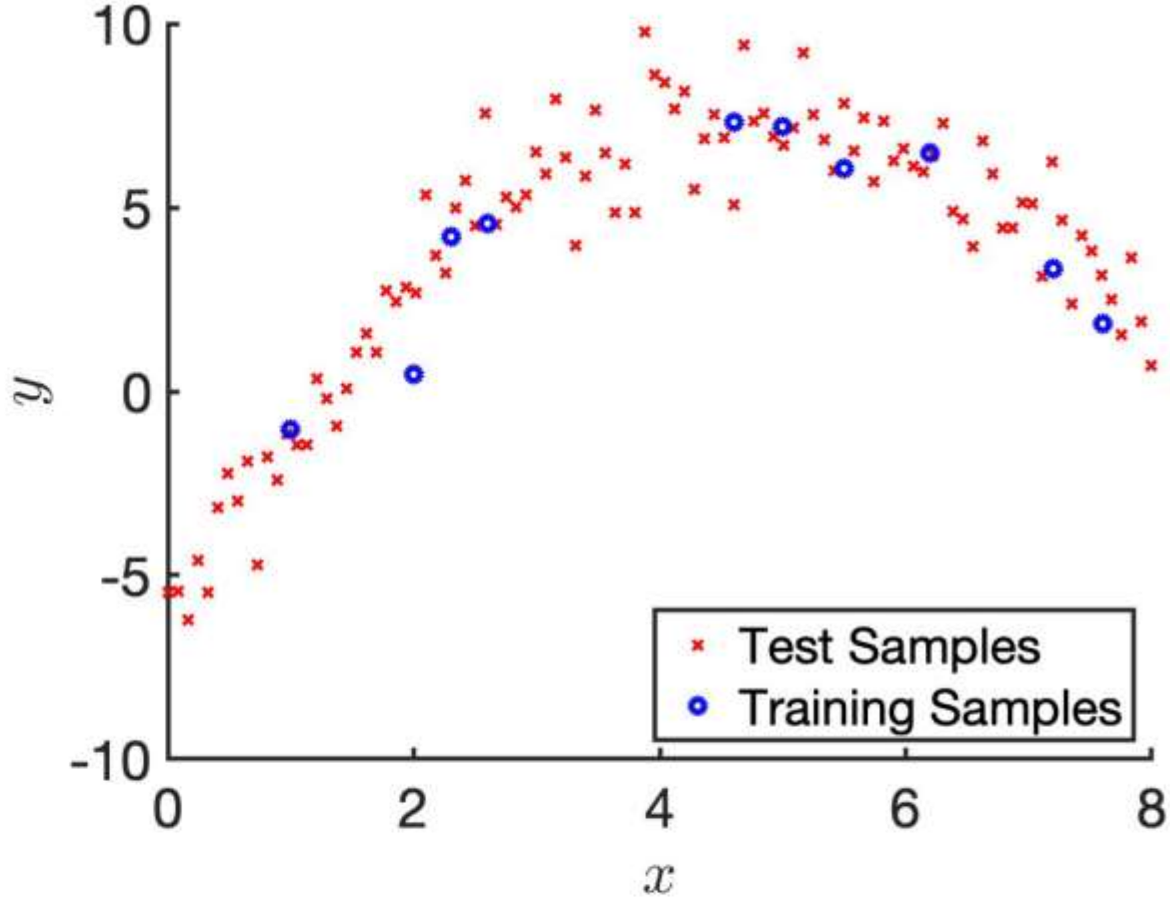
(Si

Might want to fit an affine model instead

Predicts that an earthquake of magnitude 9.0 occurs once every 500 years

Could have reinforced the buildings

Overfitting Example



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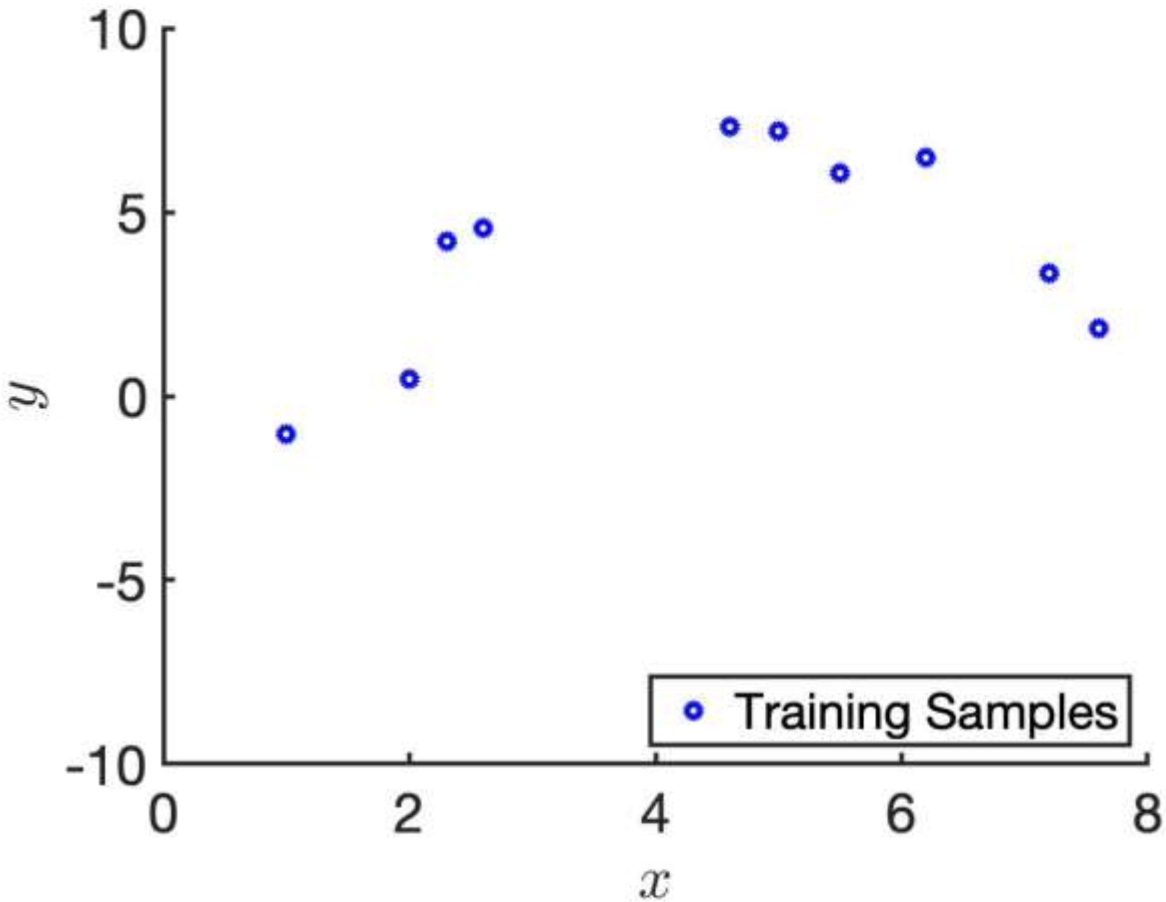

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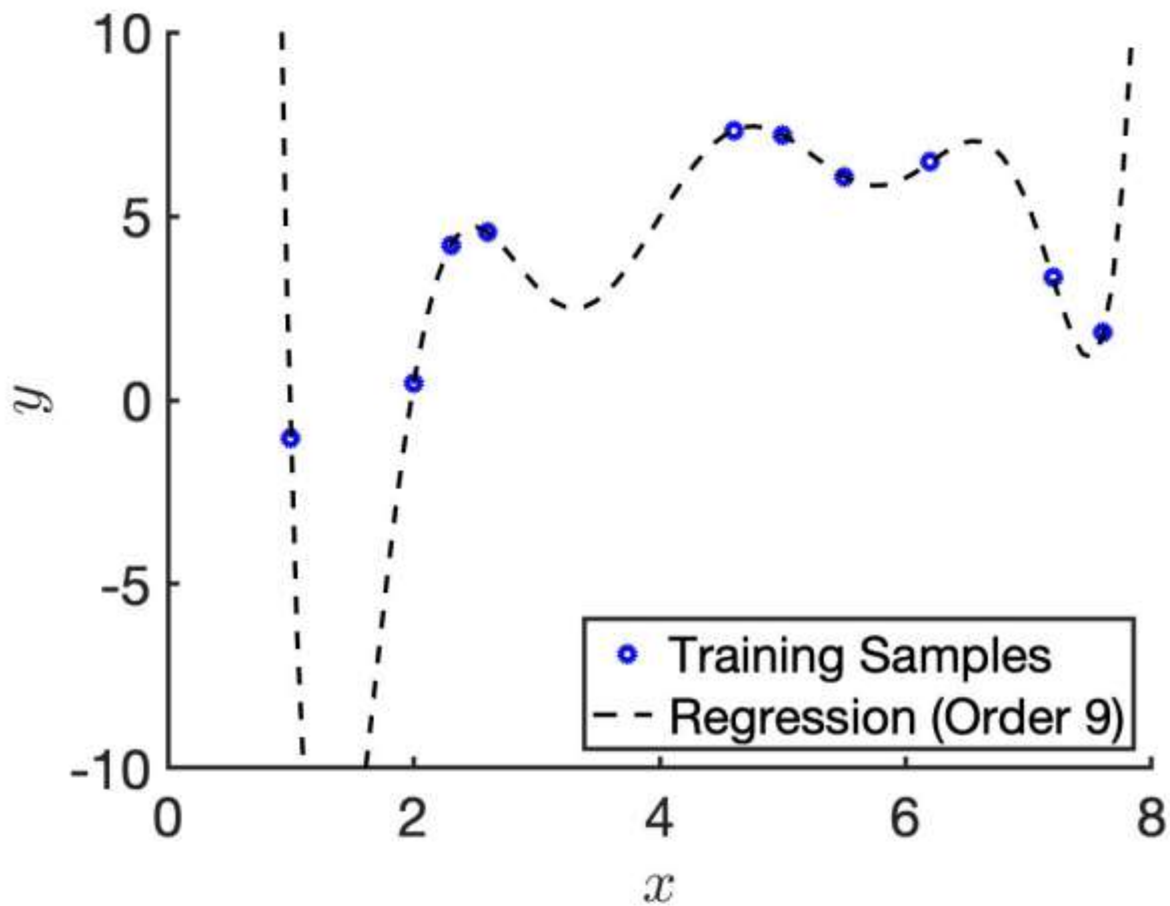
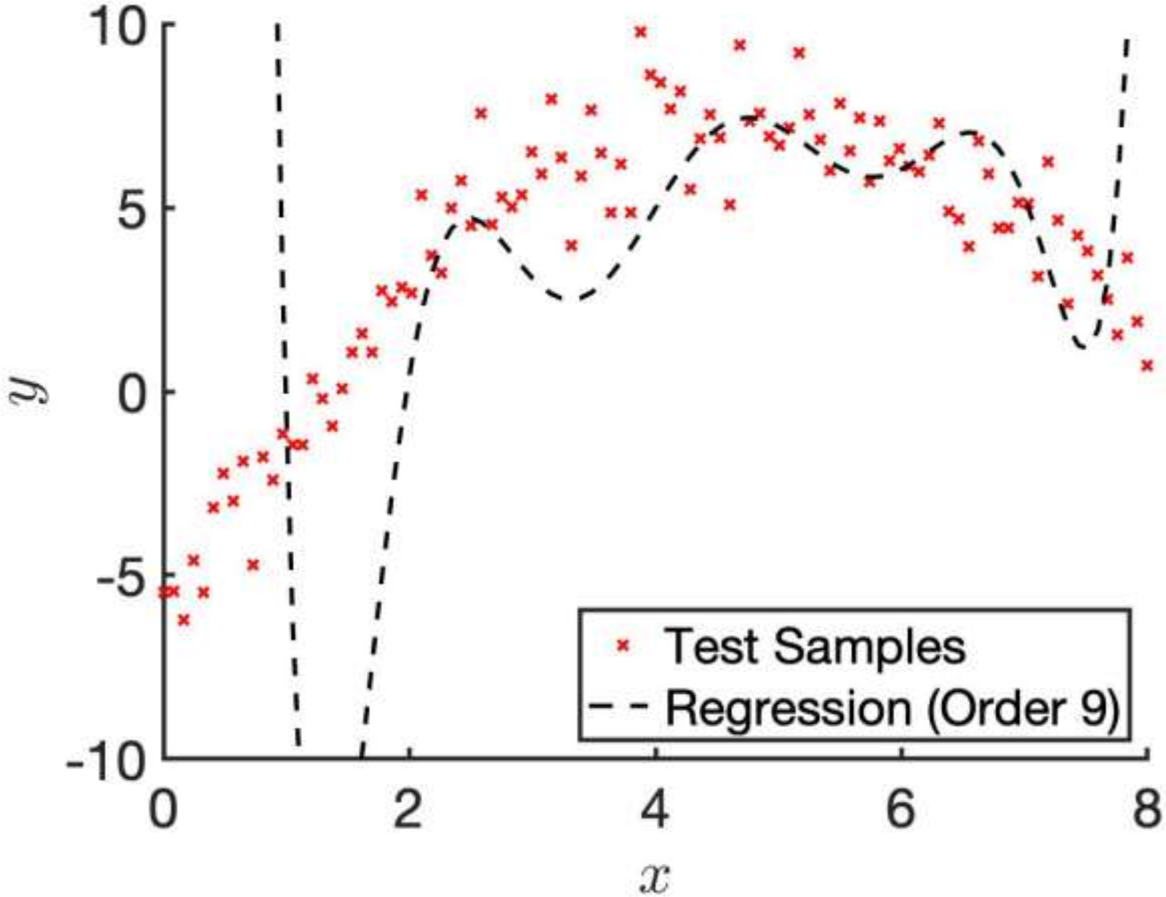


	Training Set Fit	
Order 9	Good	

Overfitting Example



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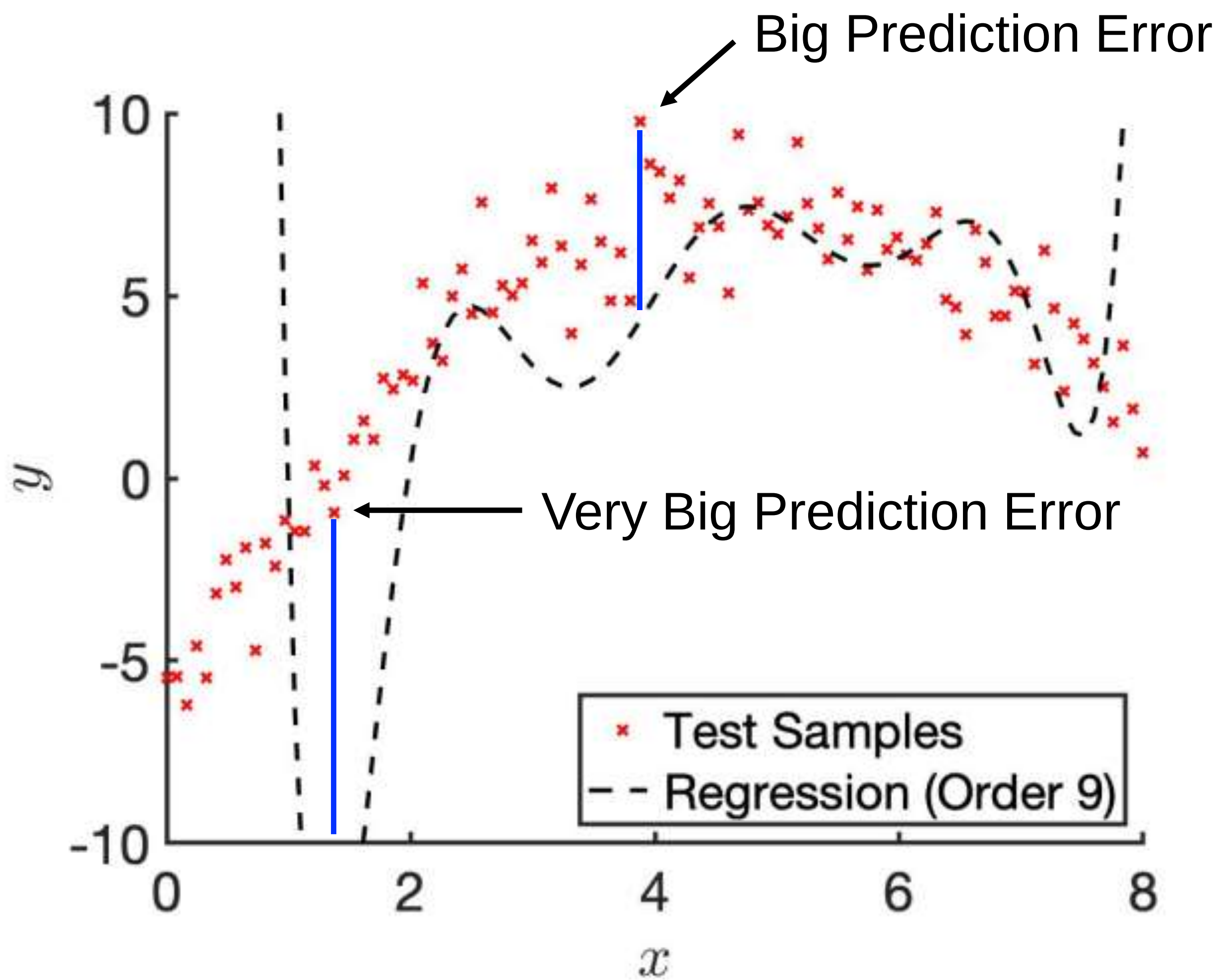

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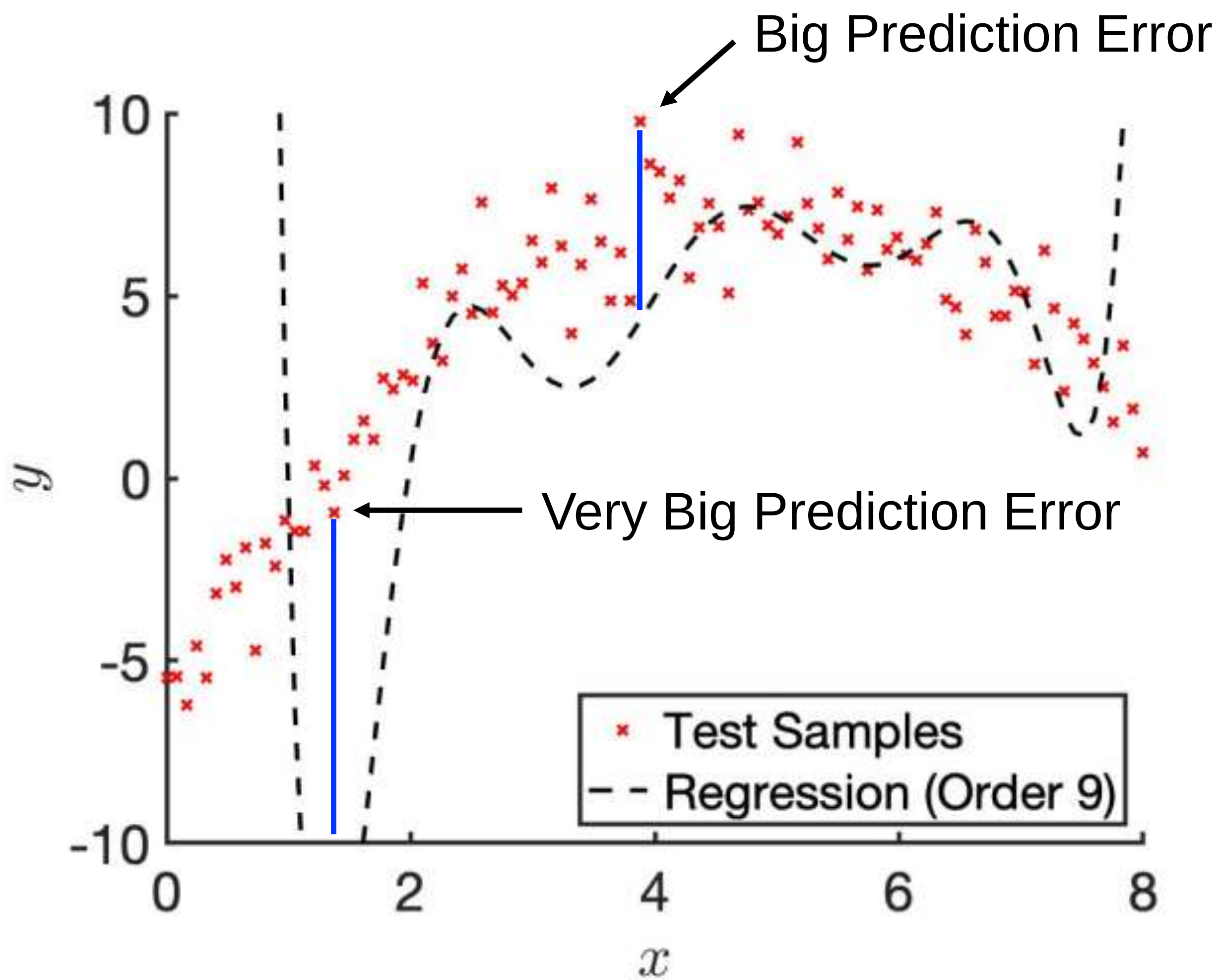
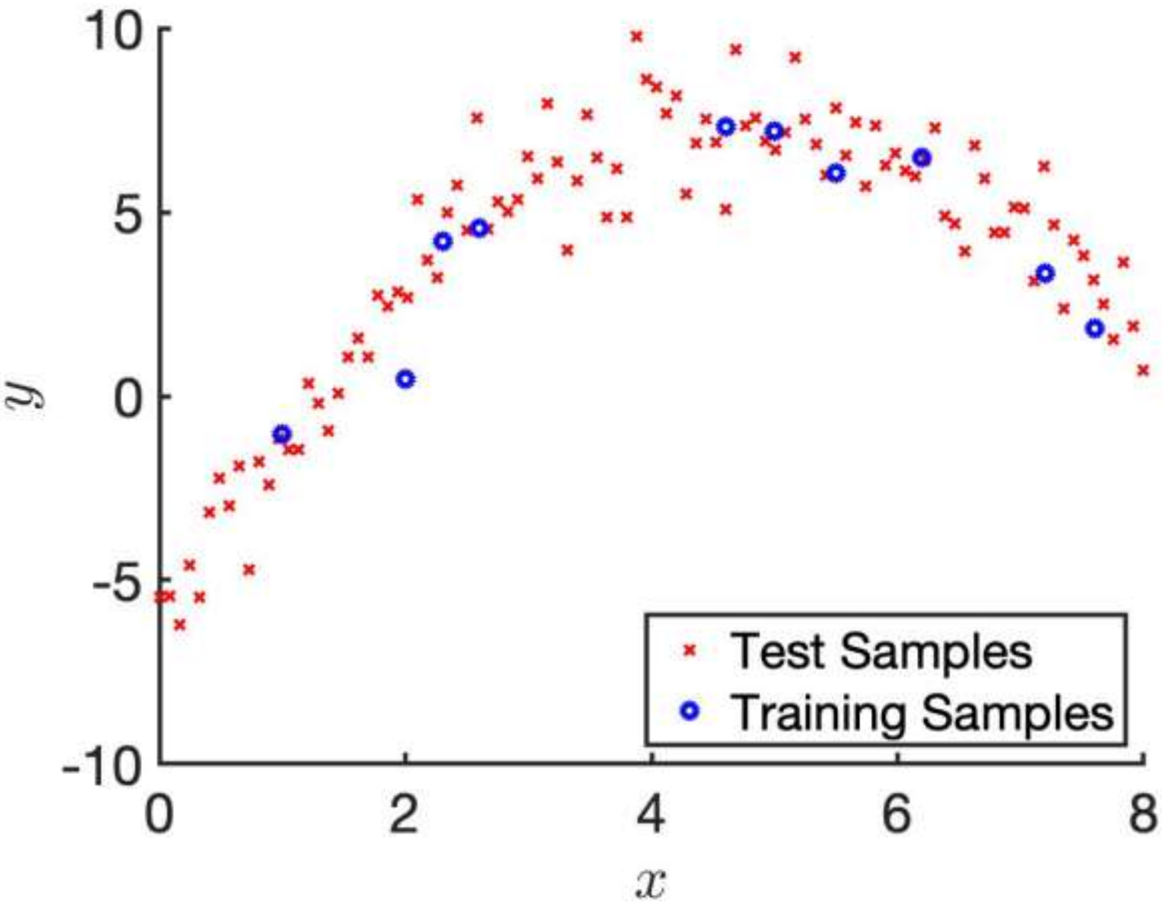
Overfitting Example



- If we take one of the blue lines and compute the square of its length, this is called **"squared error" for that particular data point**
- If we average squared errors across all the red crosses, it's called **mean squared error (MSE)** in the test set

Underfitting Example



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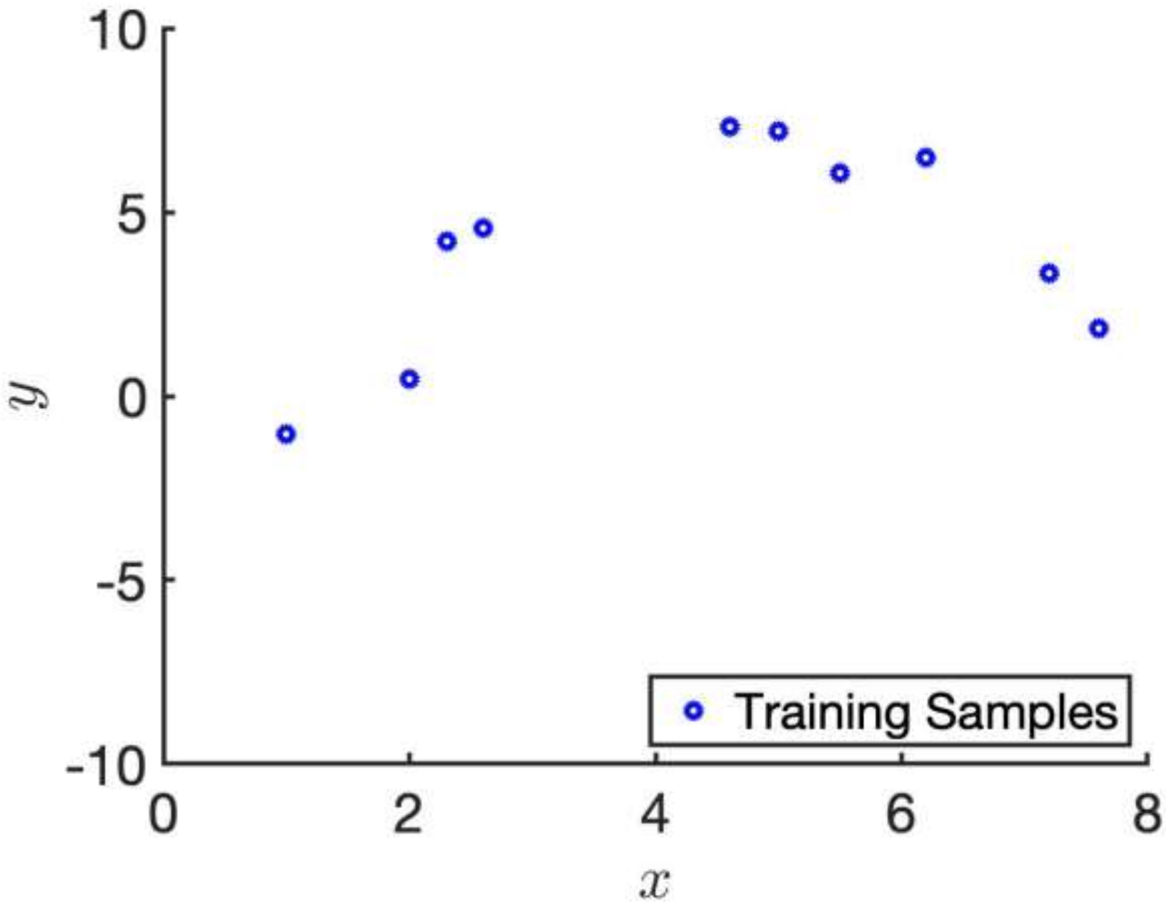

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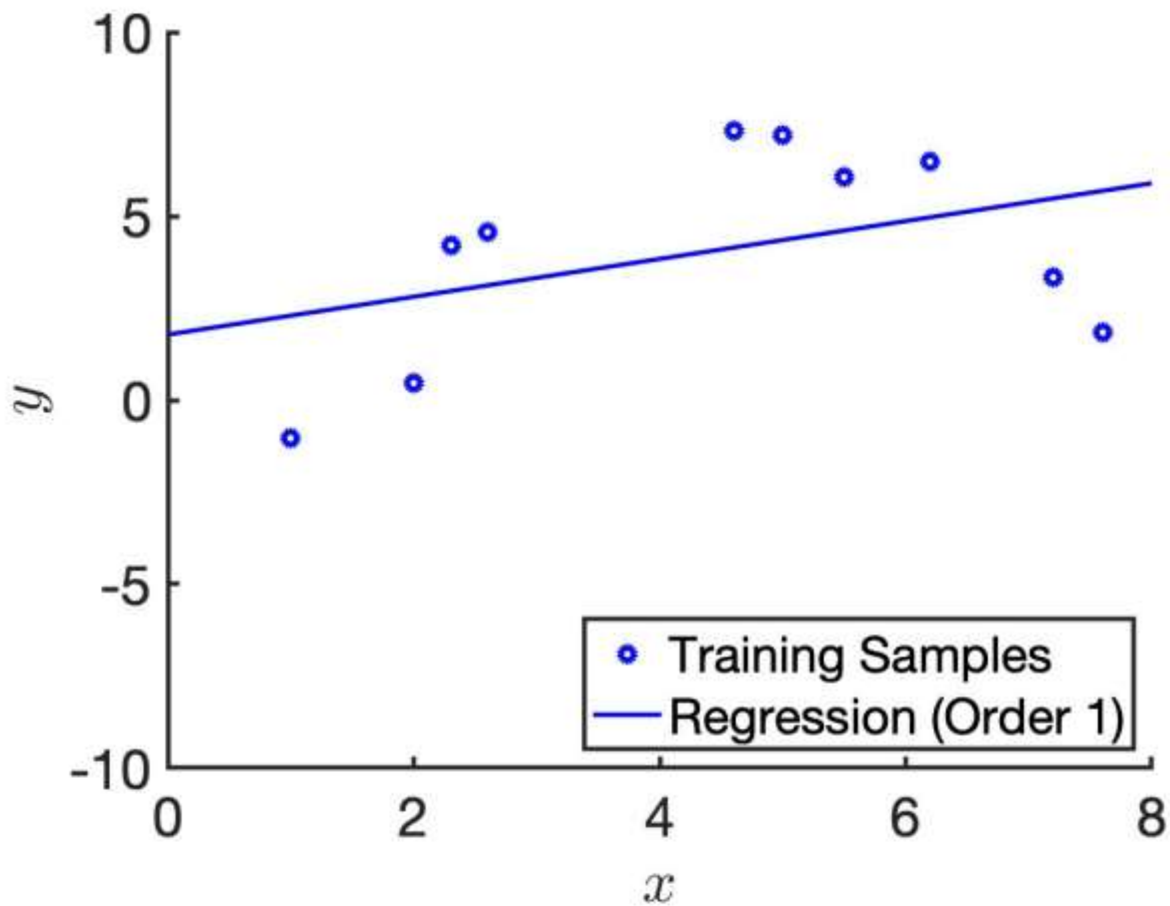

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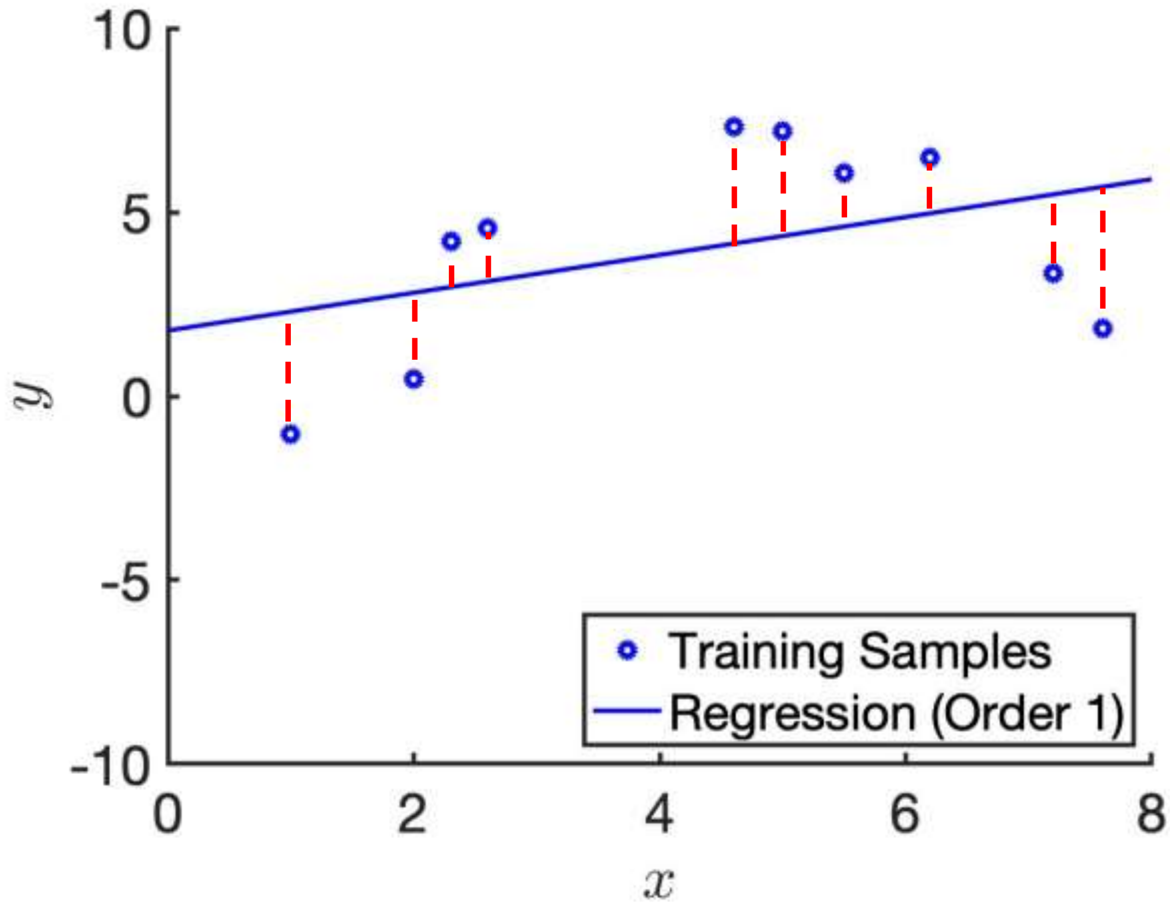

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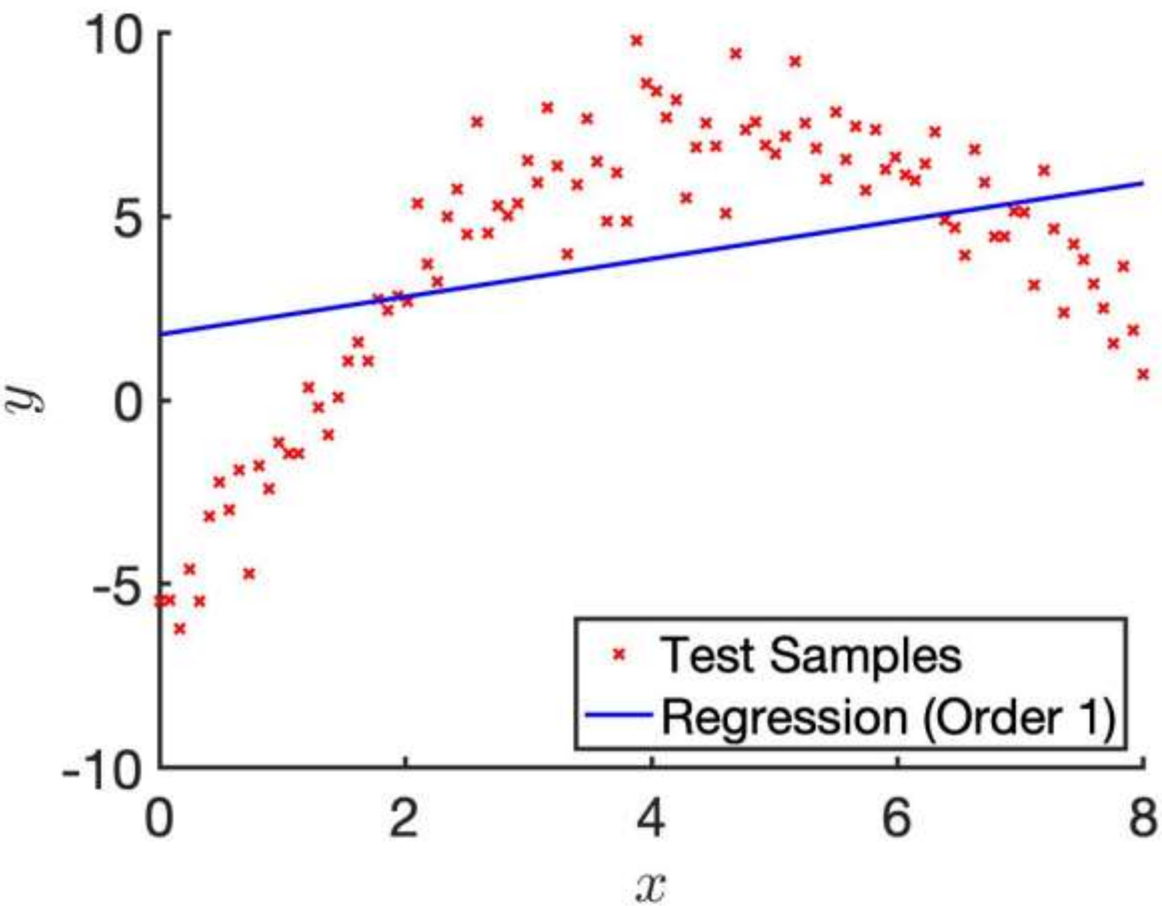

	Training Set Fit	Test Set Fit
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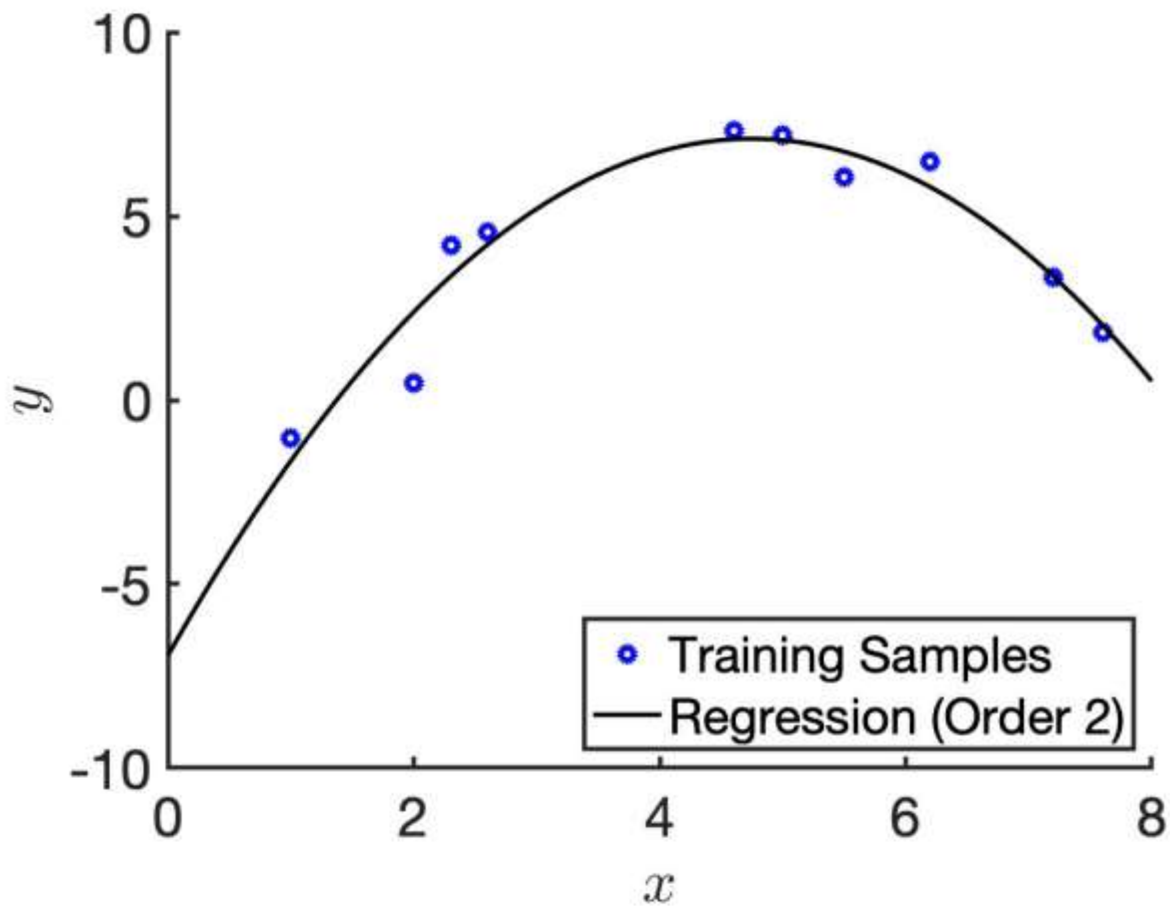
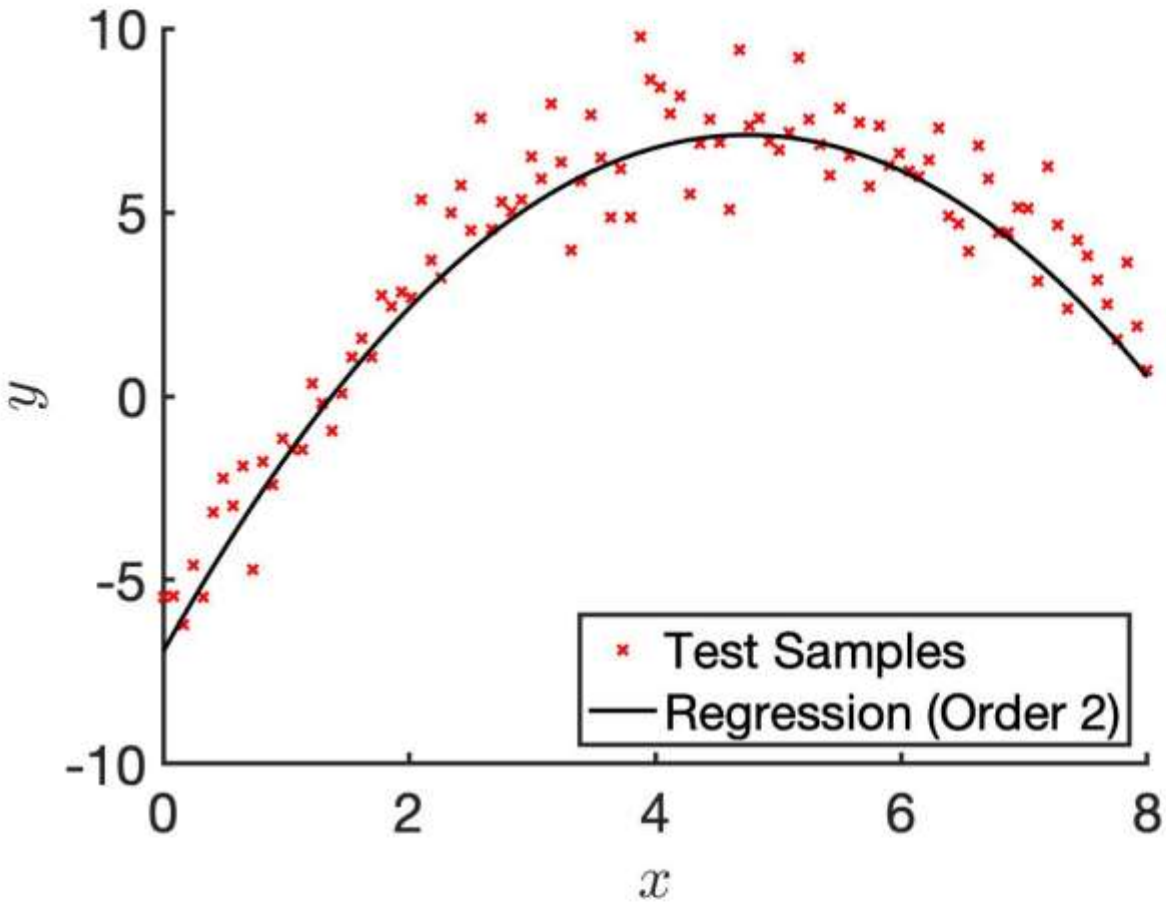
“Just Nice”



	Training Set Fit	Test Set Fit
Order 9	Good	Bad
Order 1	Bad	Bad
Order 2	Good	

"Just Nice"



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Overfitting & Underfitting

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Overfitting → Order 9

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  - Previous example: Fit order 9 polynomial to 10 data points
- **Reason 2**
  - Too many features but number of training samples too small
  - Even linear model can overfit, e.g., linear model with 9 input features (i.e., w is 10-D) and 10 data points in training set => data might not be enough to estimate 10 unknowns <u>well</u>

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- **Solutions**
  - – Use **simpler models** (e.g., lower order polynomial)
  - – Use **regularization** (see next part of lecture)

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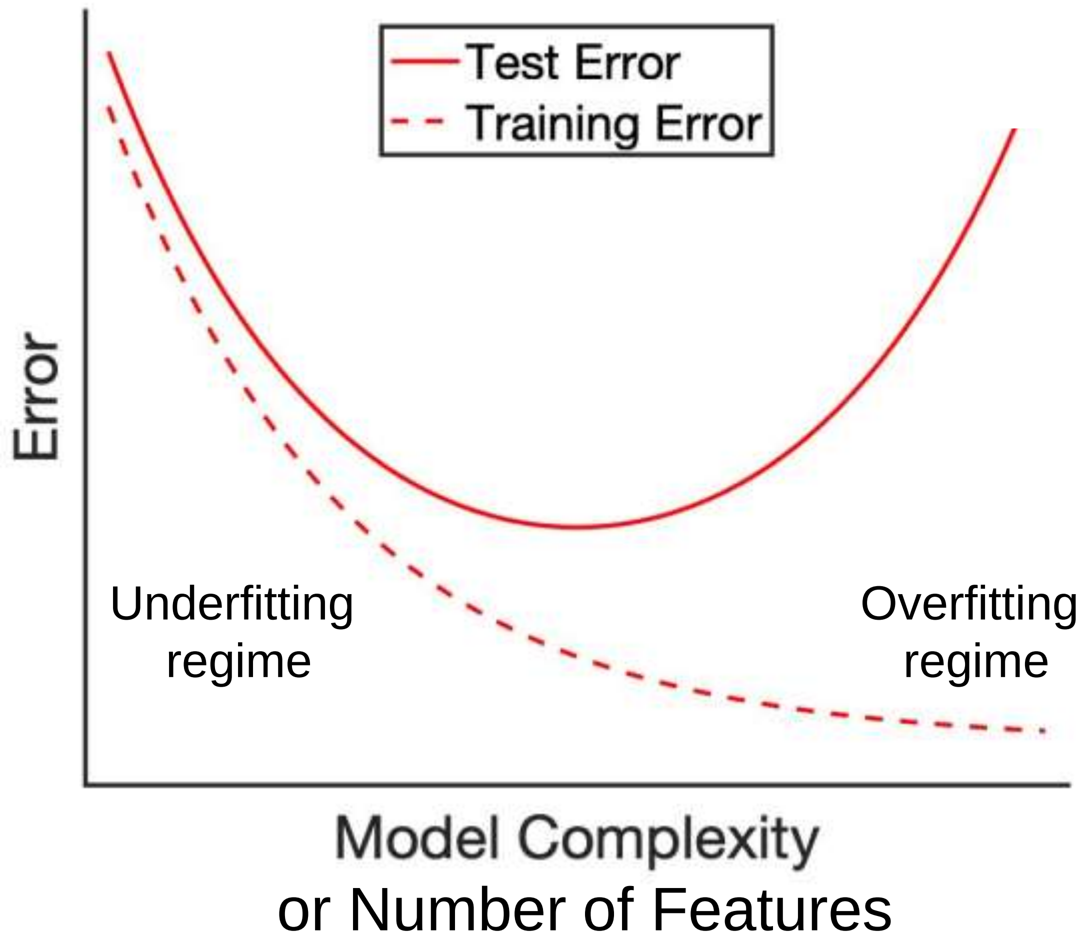
- **Reason 2**
  - Features are not informative enough
  - **Solution**: Try to develop more informative features

Overfitting / Underfitting Schematic



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- Very common mistake
  - Feature selection with test set (or full dataset) leads to inflated performance
  - Do not perform feature selection with test data

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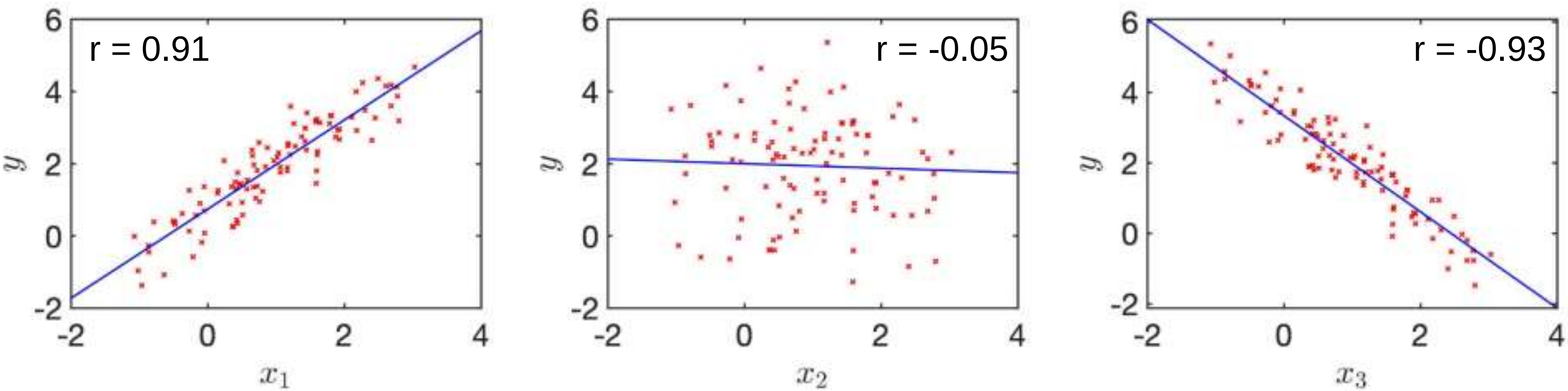

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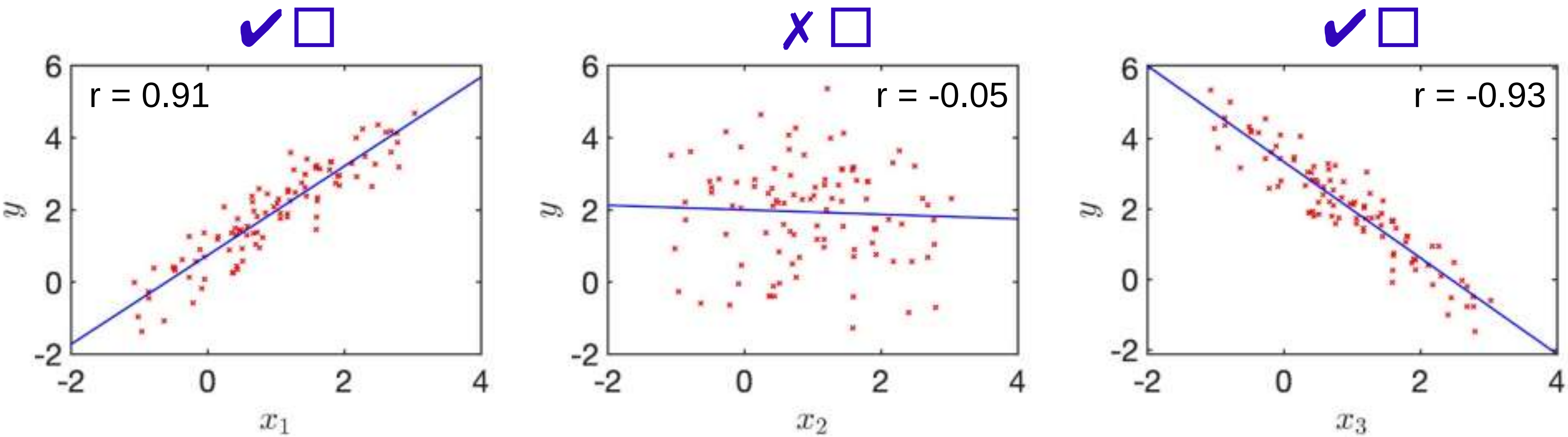

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- Other metrics besides Pearson's correlation are possible

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- For example, in previous lecture, we added $\lambda \mathbf{w}^T \mathbf{w}$:

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- For $\lambda > 0$, matrix becomes invertible (Motivation 1)

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- $\hat{\mathbf{w}}$ might also perform better in test set, i.e., reduces overfitting (Motivation 2) – will show example later

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- Consider minimization from previous slide

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Cost function quantifying data fitting error in training set

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- More generally, most machine learning algorithms can be formulated as the following optimization problem

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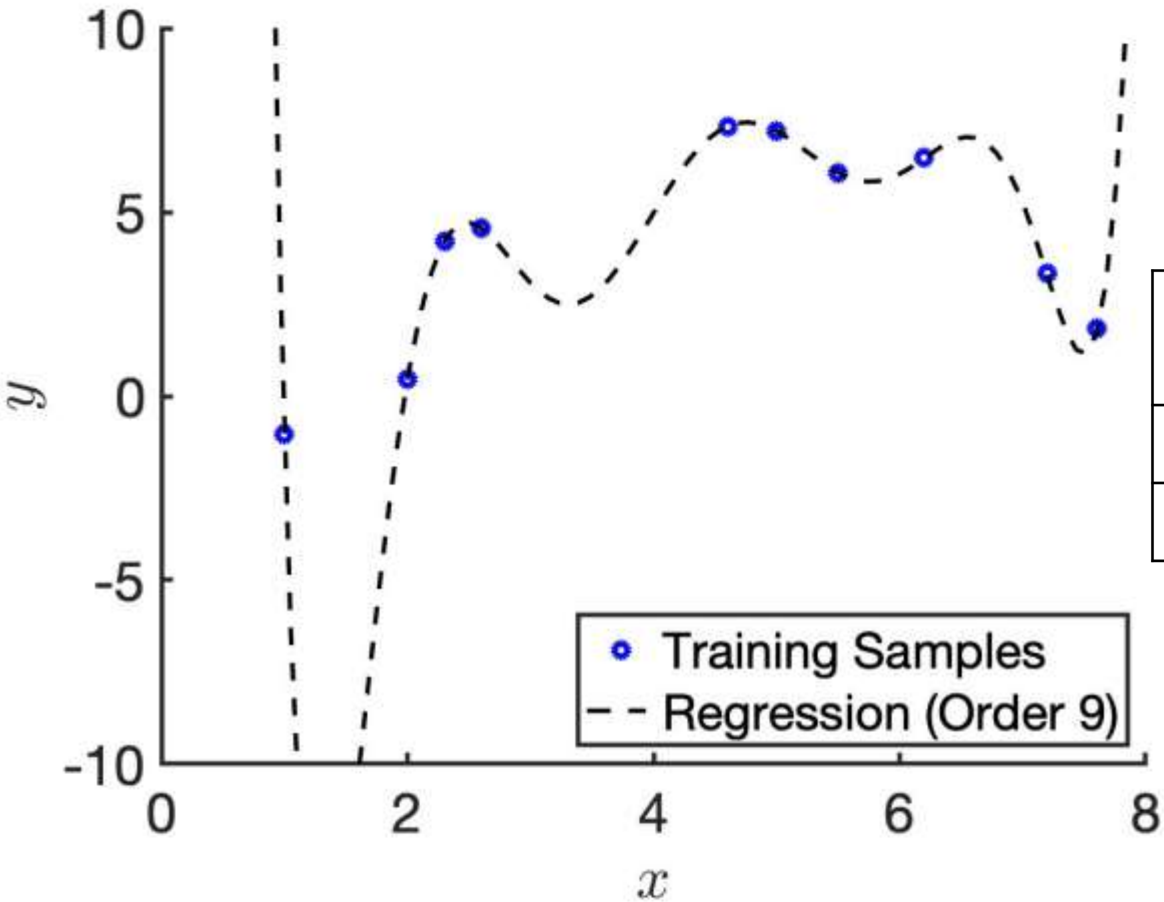
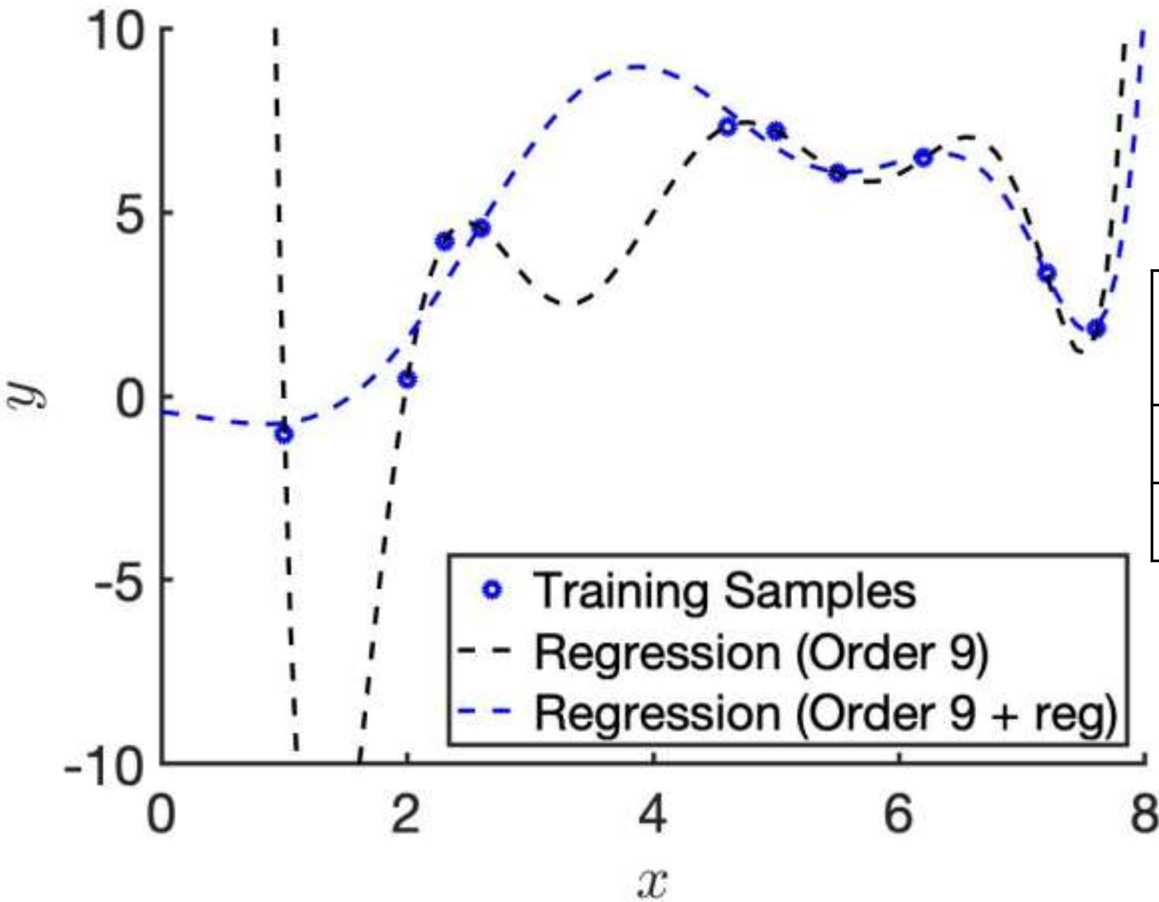
- **Regularization(w)** penalizes more complex models

Regularization Example



	Training Set Fit	Test Set Fit
Order 9	Good	Bad

Regularization Example



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Order 9	Good	Bad
Order 9, $\lambda = 1$	Good	

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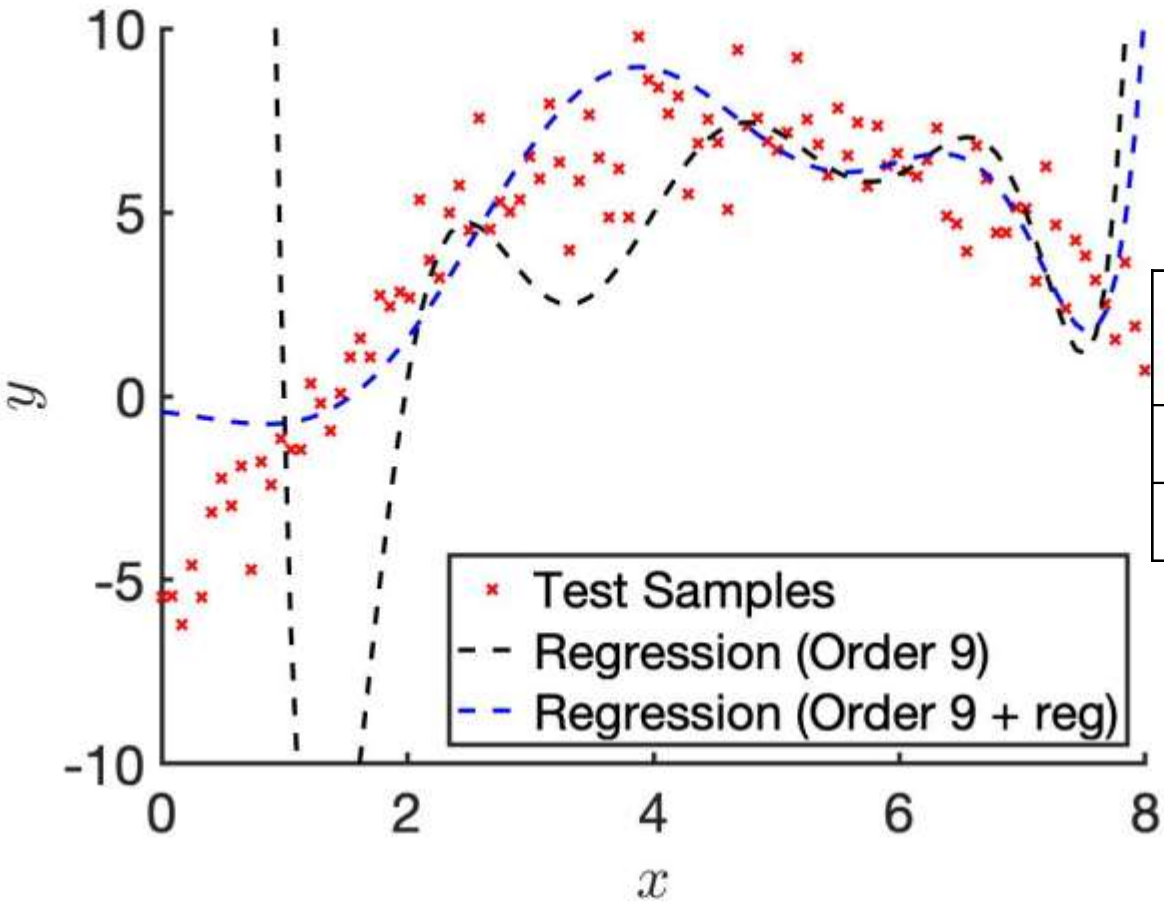

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Questions?

Bias versus Variance

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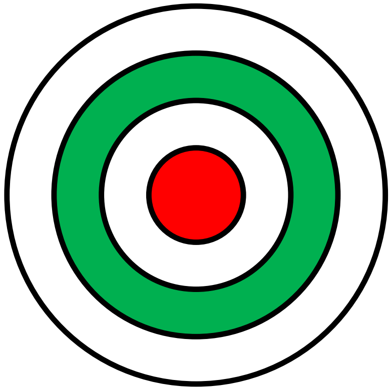

Bias versus Variance

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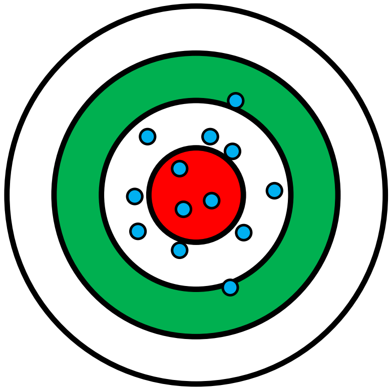
High Variance

Low Bias

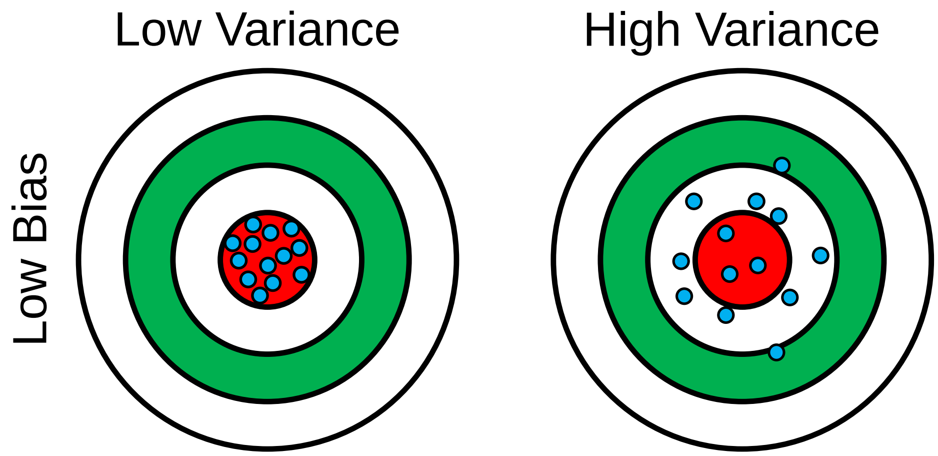


Low Bias: blue predictions on average close to red target
High Variance: large variability among predictions

Bias versus Variance

- Suppose we are trying to predict red target below:

Low Bias: blue predictions on average close to red target
Low Variance: low variability among predictions



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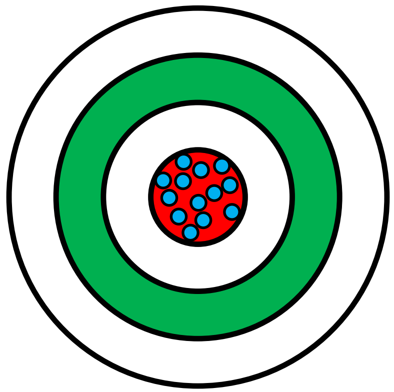
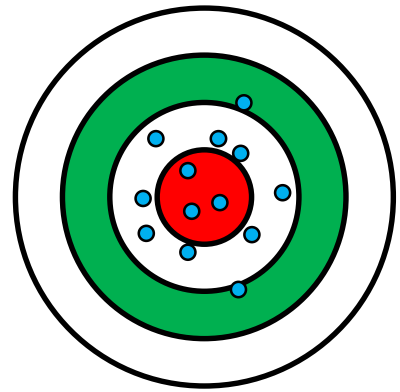
Low Bias





Low Bias: blue predictions on average close to red target
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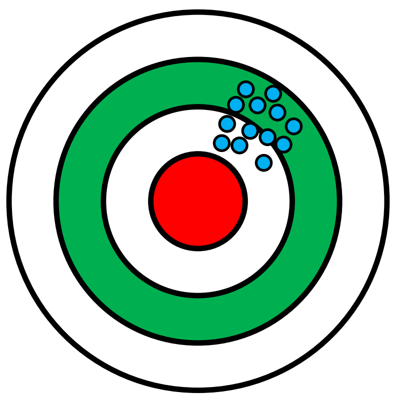
High Bias: blue predictions on average not close to red target
Low Variance: Low variability among predictions

High Bias



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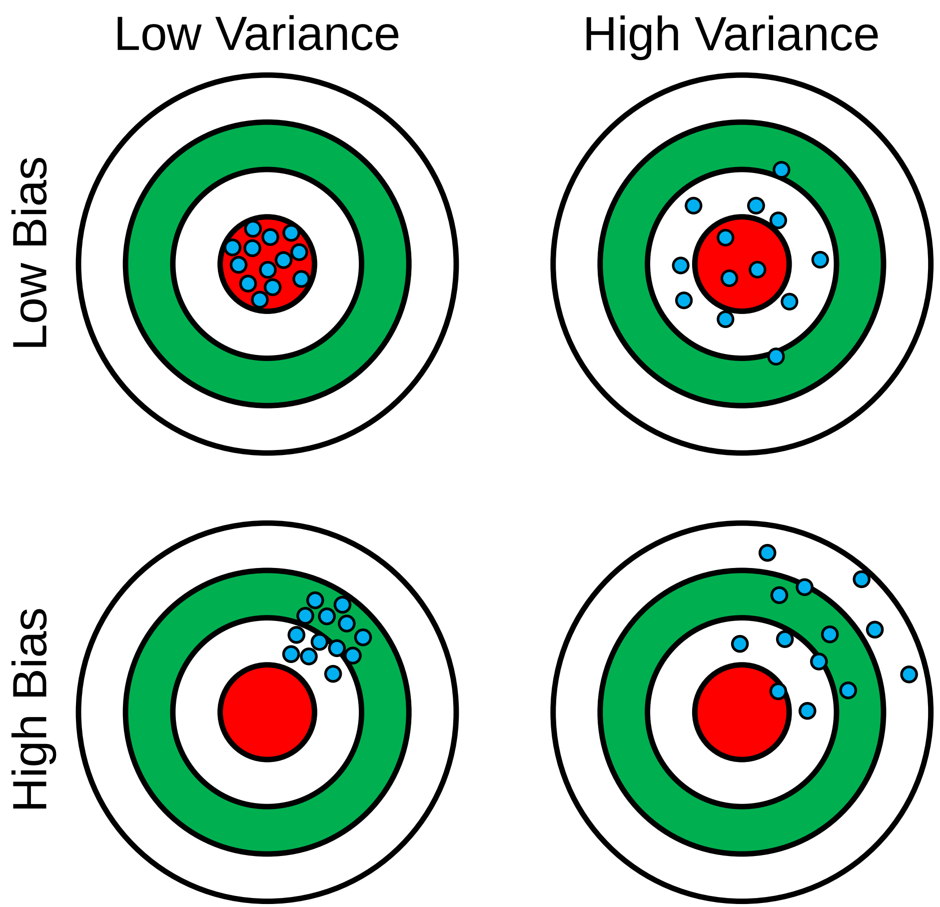

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Bias + Variance Trade off

- Test error = Bias Squared + Variance + Irreducible Noise

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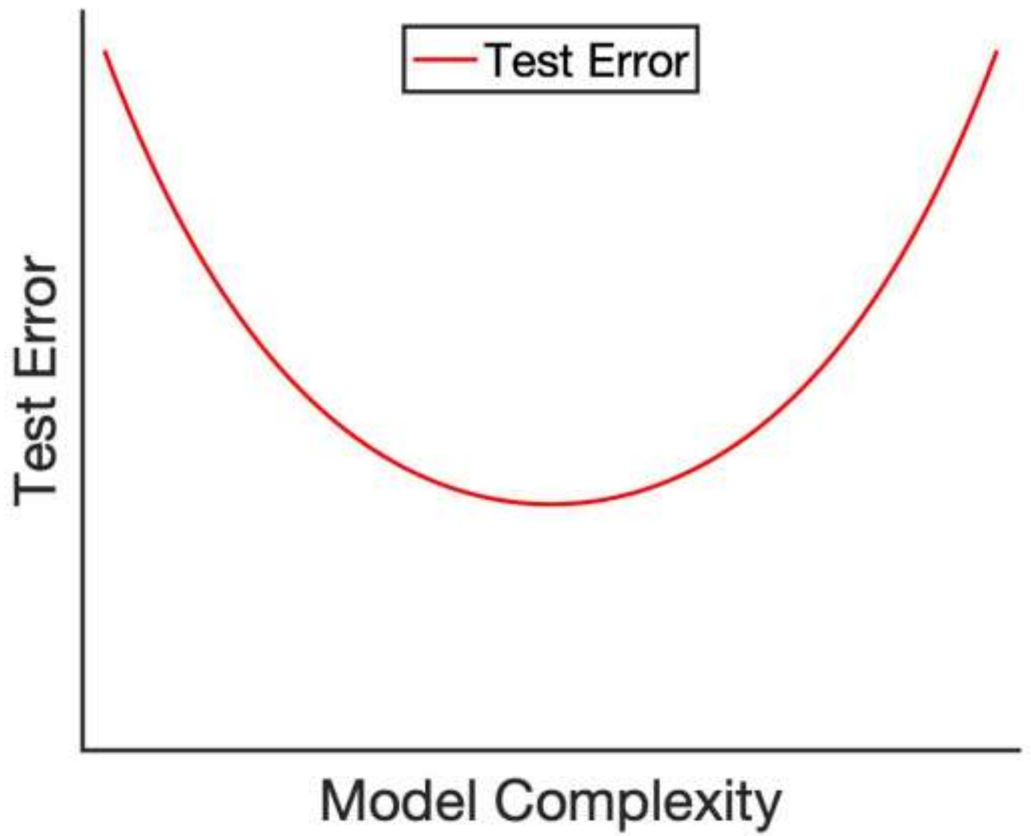

or Number of Features

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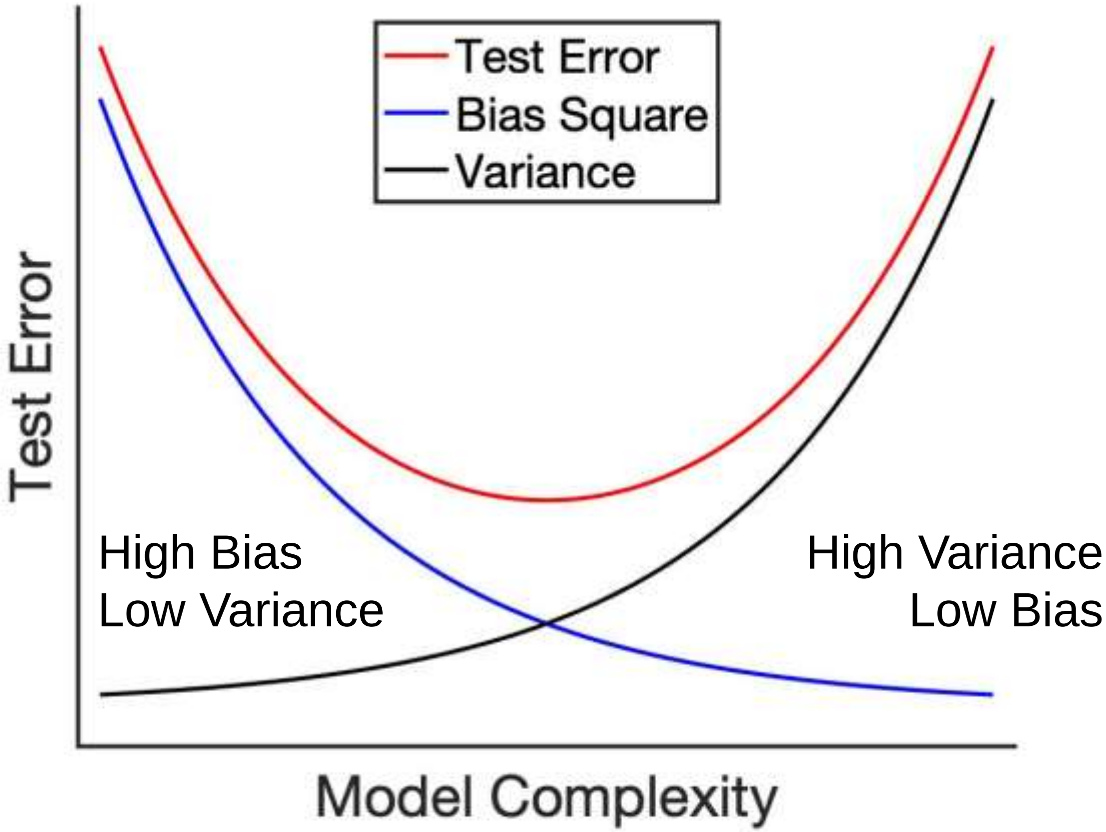

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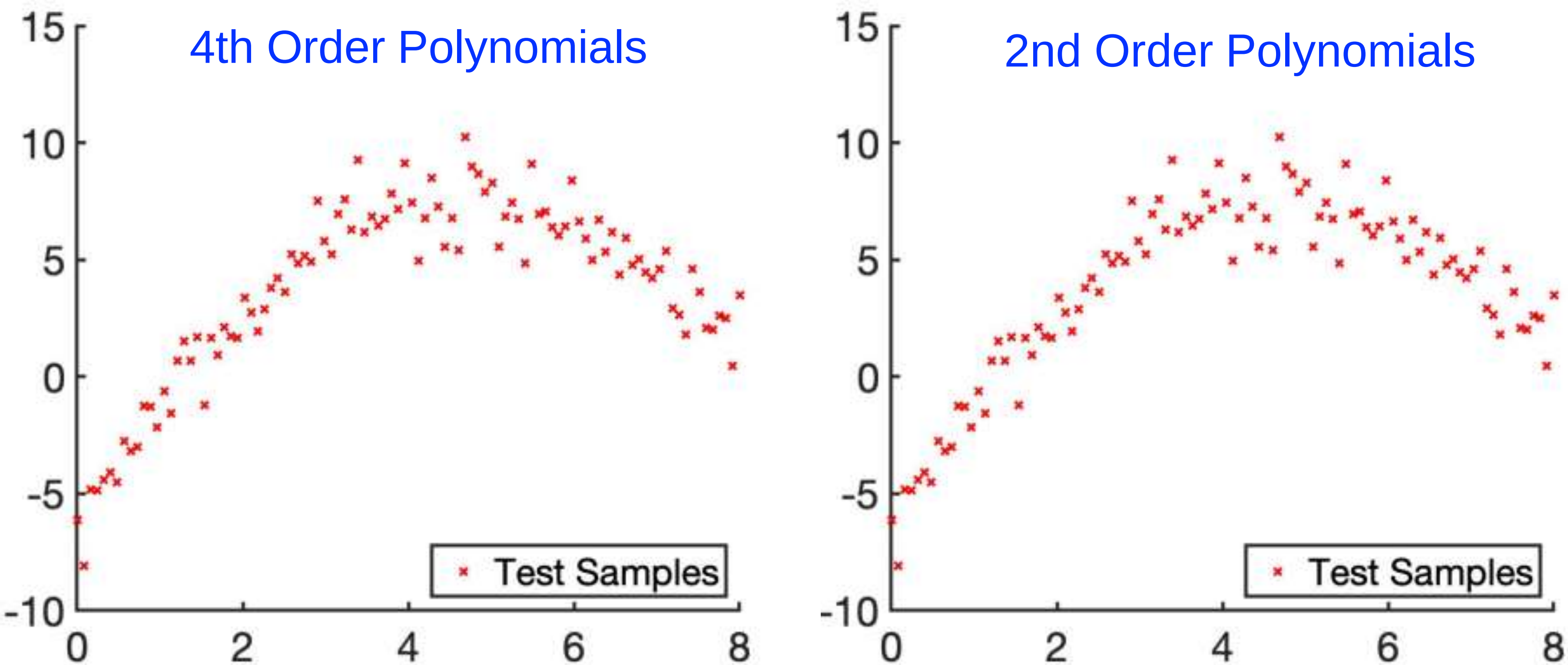
Bias + Variance Example

- Simulate data from order 2 polynomial (+ noise)
- Randomly sample 10 training samples each time



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- Fit with order 2 polynomial
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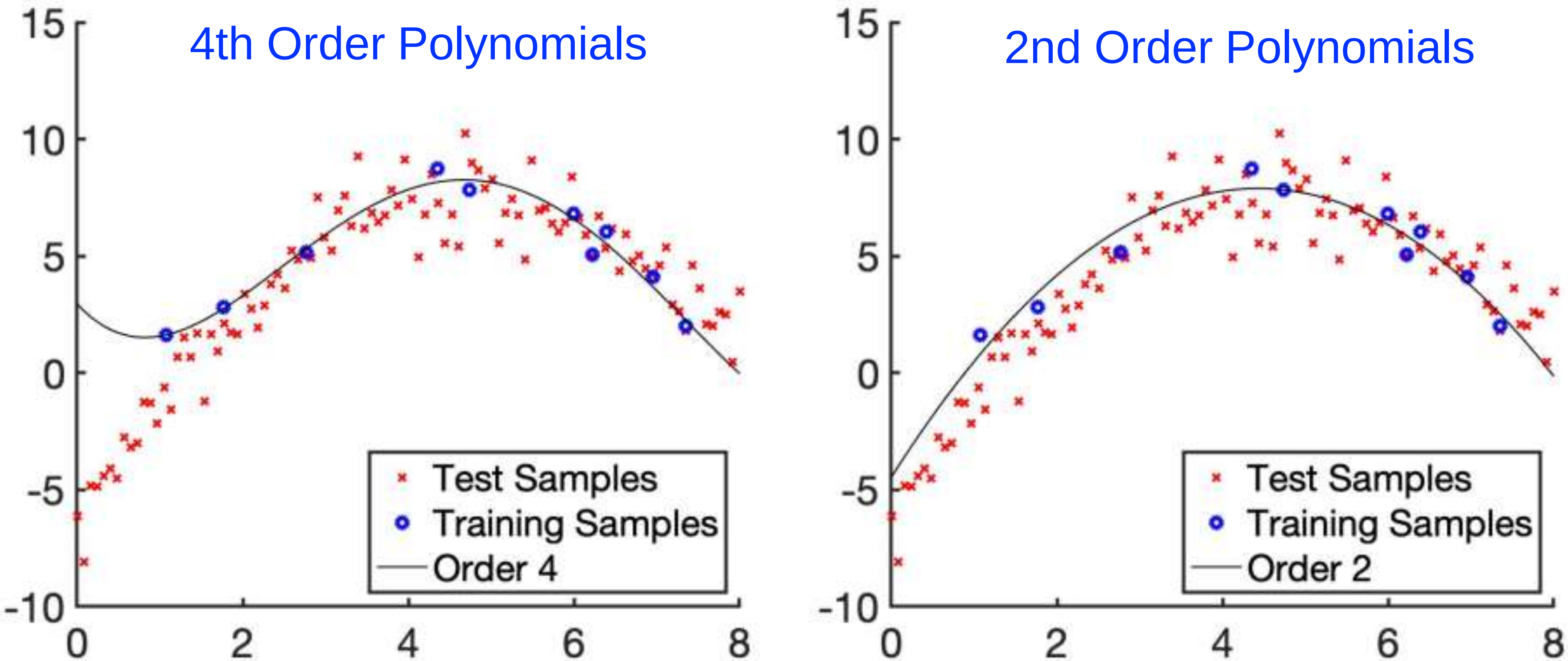

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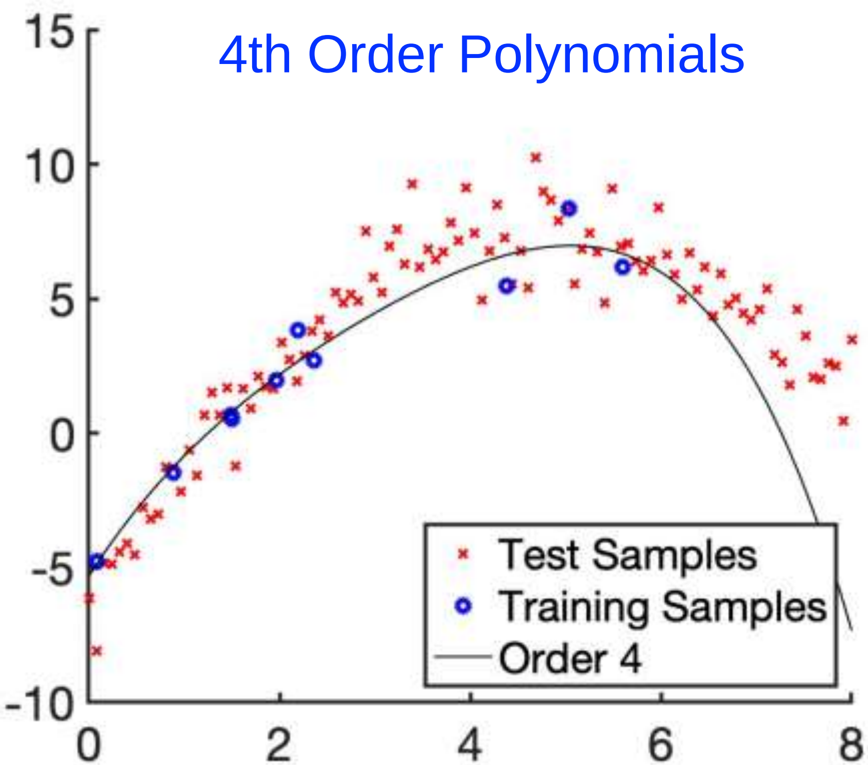

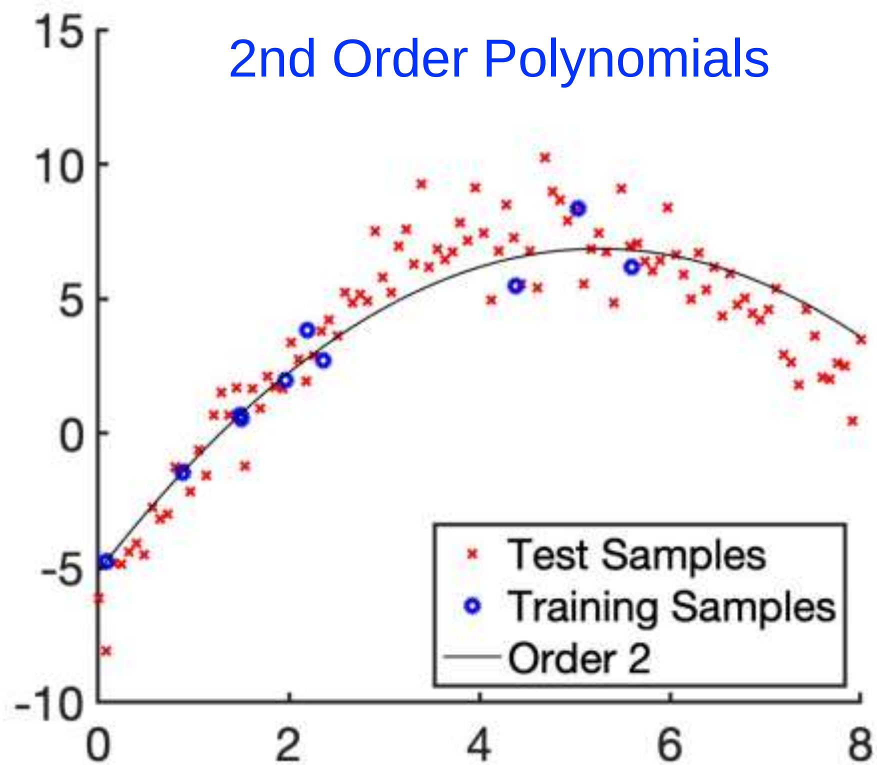

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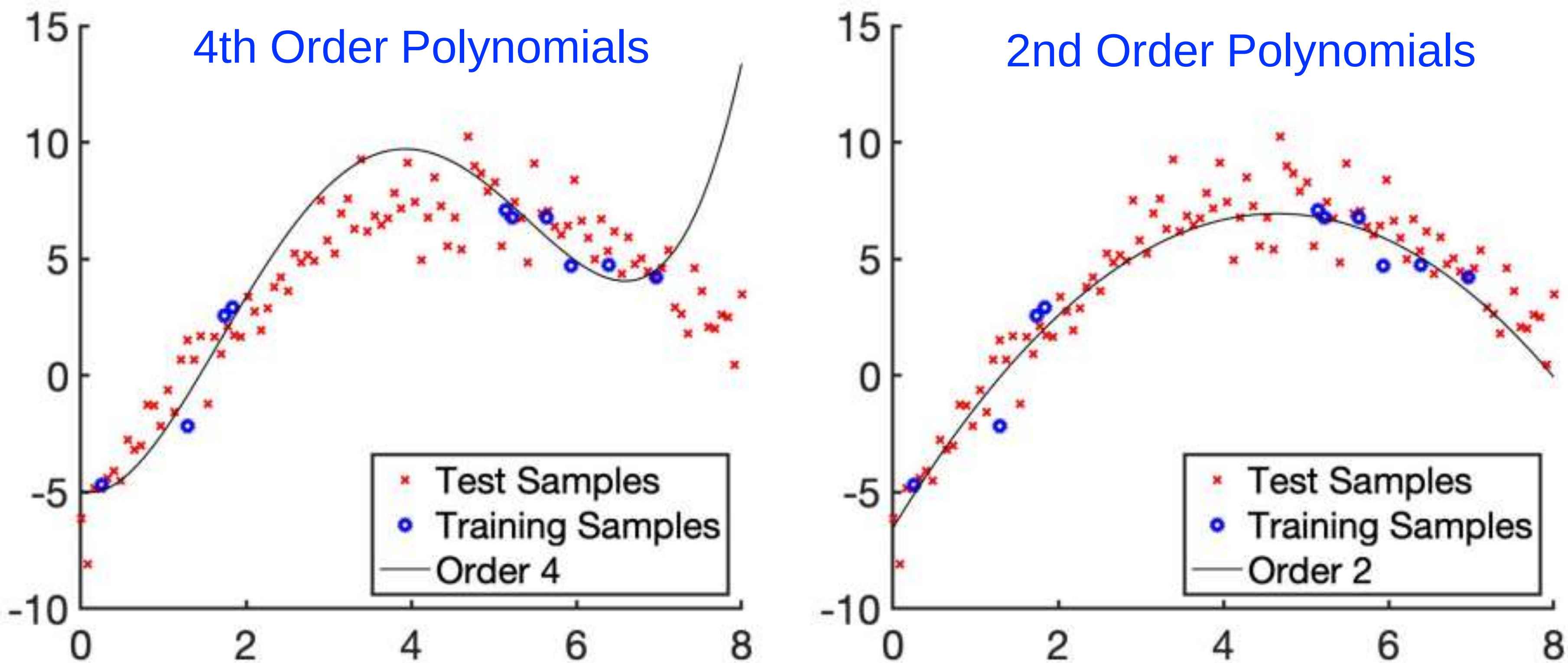

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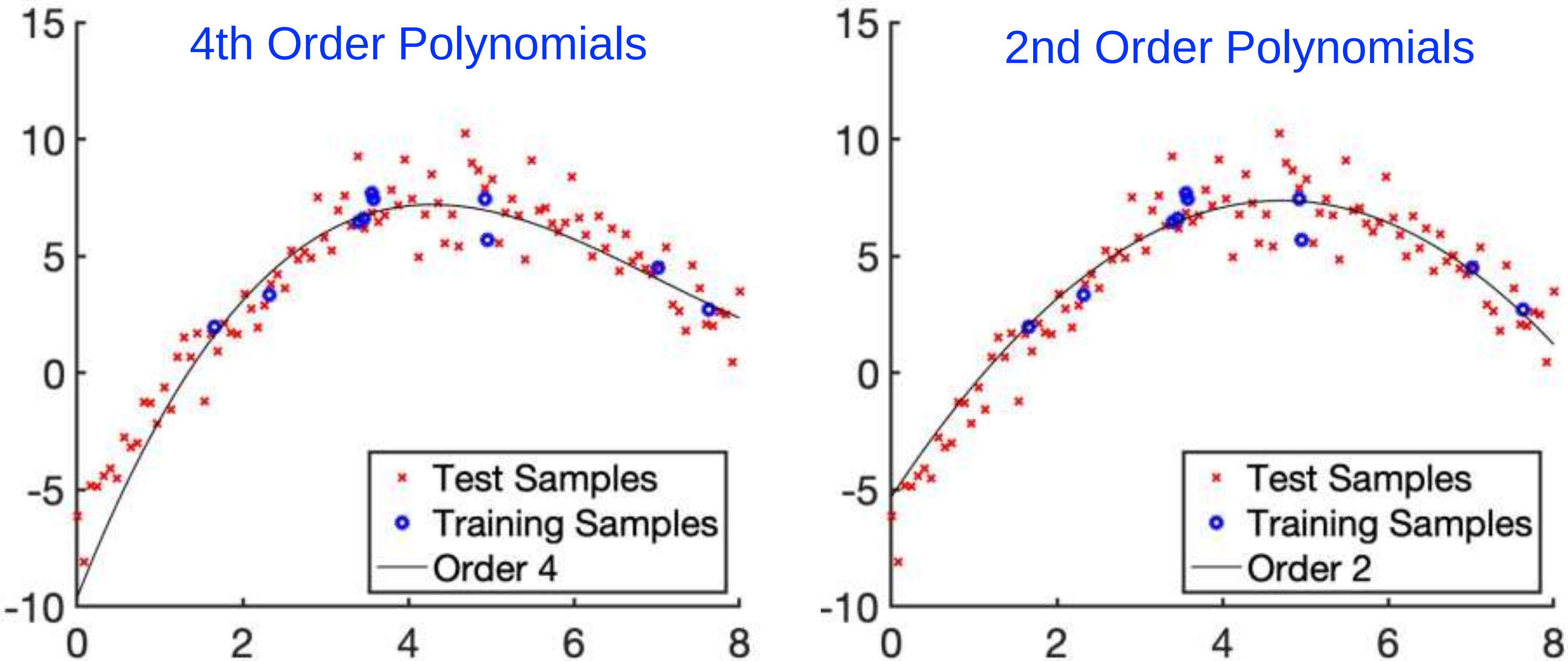

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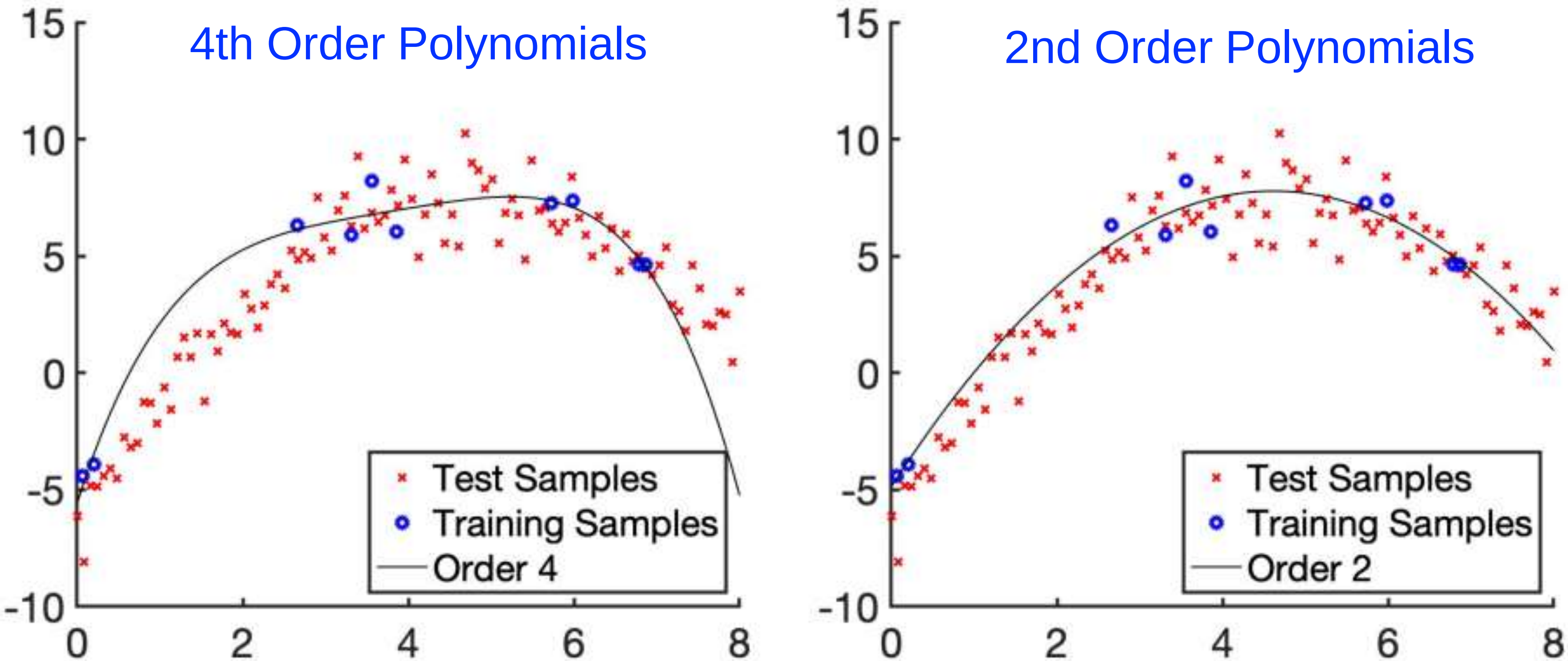

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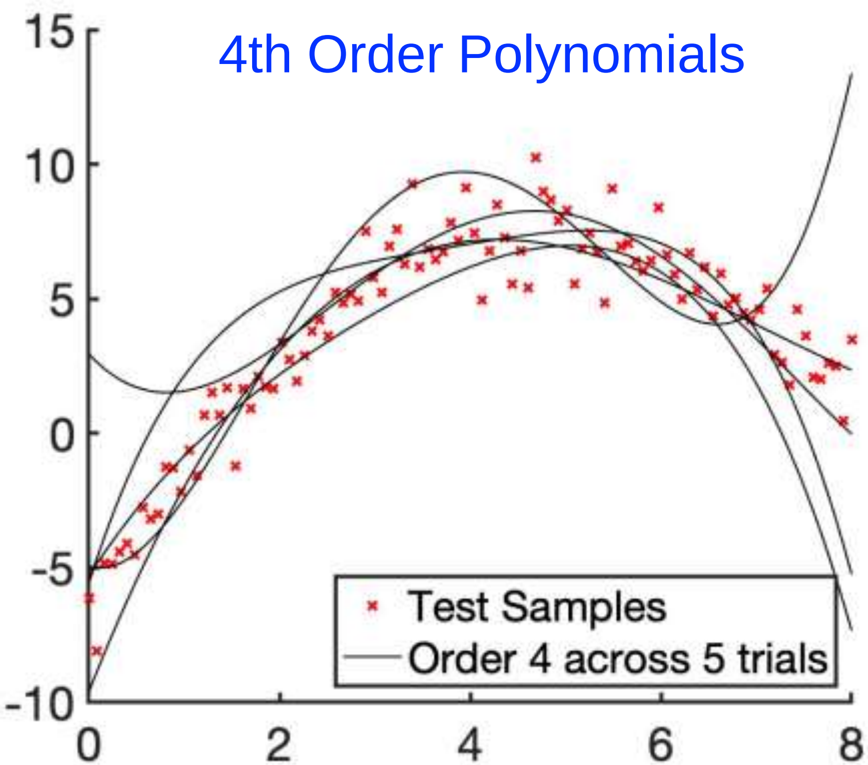
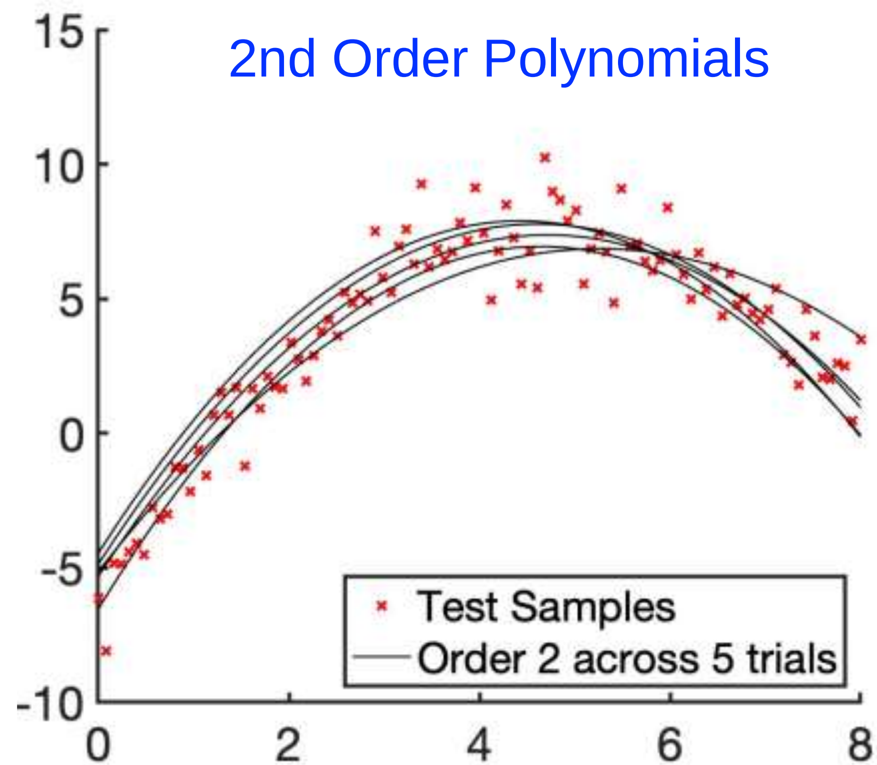
- Fit with order 4 polynomial: high variance





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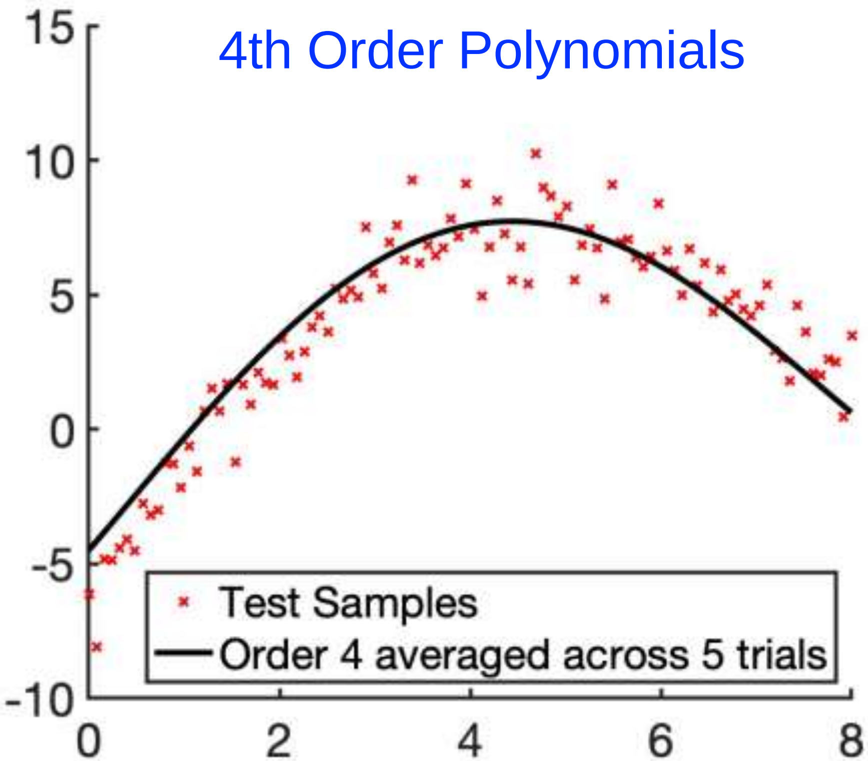

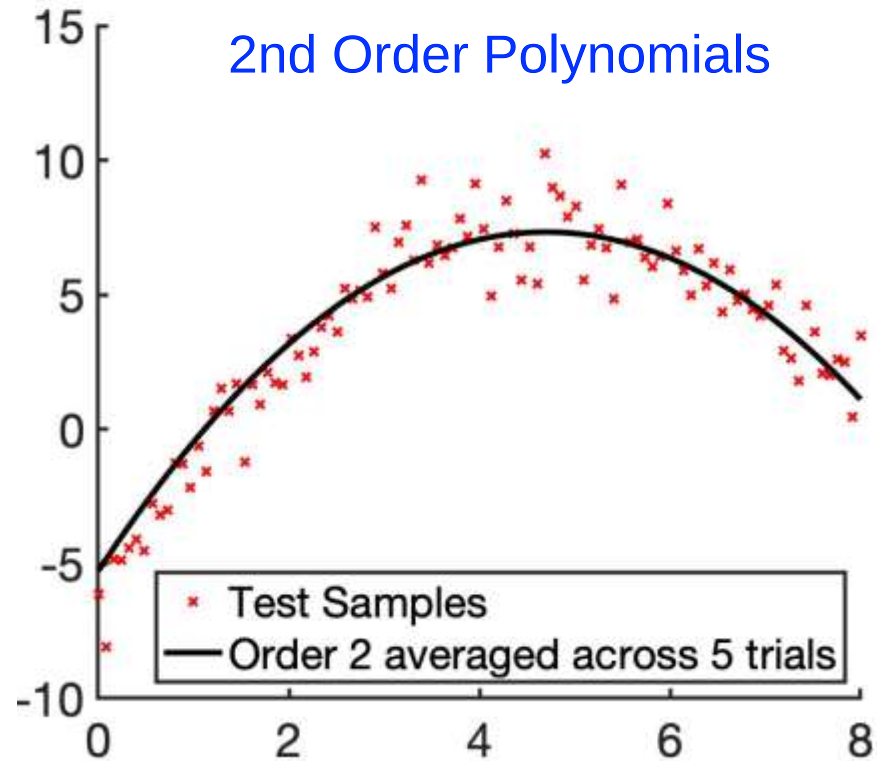

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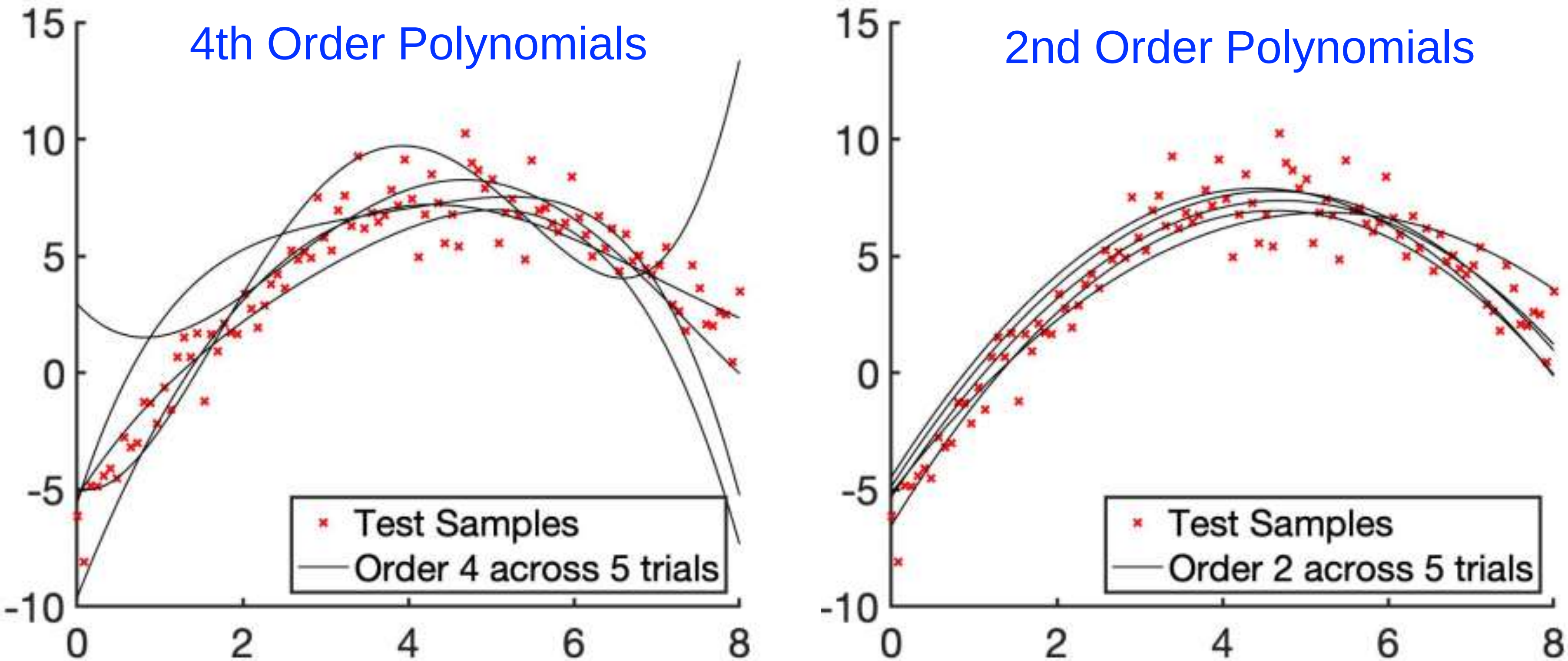
Order 2 Achieves Lower Test Error



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- E_D is expectation with respect to $p(D)$: think of this as averaging across ∞ trials

Bias-Variance Decomposition Theorem

- Think of E_D as averaging across ∞ trials

- See proof in extra uploaded material (won't be tested)

Bias-Variance Decomposition Theorem

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- According to the Bias-Variance Decomposition Theorem, the mean squared error for a new test sample x is given by

$$E_D\left[\left(y(x) - \underbrace{\hat{f}_D(x)}_{\hat{y}_{test}}\right)^2\right]$$

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$$\text{Bias}(\hat{f}) = \hat{f}_{avg}(x) - f(x),$$

and

$$\text{Var}(\hat{f}) = E_D\left[\left(\hat{f}_D(x) - \hat{f}_{avg}(x)\right)^2\right]$$

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Numerical Example of Bias and Variance Tradeoff I

- We have randomly sampled a training set $D = \{(\mathbf{x}_i, y_i)\}_{i=1}^m$ from a probability distribution $p(D)$.
- Using D, we training a regression model to predict y from $\mathbf{x}$.
- For simplicity, say that $\mathbf{x}$ and $\mathbf{x}_i$ are one-dimensional, so we write them as x and x_i for brevity.
- We repeat this process of sampling the dataset from $p(D)$ a total of 4 times, resulting in 4 trained models

$$\hat{f}_{D_1}, \hat{f}_{D_2}, \hat{f}_{D_3}, \hat{f}_{D_4}$$

  based on the datasets D_1, D_2, D_3, D_4.
- We have a new test sample $x_{\text{new}} = 3$ whose (unknown) target is $y_{\text{new}} = f(x_{\text{new}}) = 7.5$.
- The function $f(x)$ represents the real/true relation between y and x.

Numerical Example of Bias and Variance Tradeoff II

- Suppose now the predictions of x_{new} from $\hat{f}_{D_1}, \hat{f}_{D_2}, \hat{f}_{D_3}, \hat{f}_{D_4}$ are $\hat{y}_{\text{new},1} = 6$, $\hat{y}_{\text{new},2} = 7$, $\hat{y}_{\text{new},3} = 7$, $\hat{y}_{\text{new},4} = 8$ respectively. That is

$$
\begin{aligned}
\hat{y}_{\text{new},1} &= \hat{f}_{D_1}(x_{\text{new}}) = \hat{f}_{D_1}(3) = 6 \\
\hat{y}_{\text{new},2} &= \hat{f}_{D_2}(x_{\text{new}}) = \hat{f}_{D_2}(3) = 7 \\
\hat{y}_{\text{new},3} &= \hat{f}_{D_3}(x_{\text{new}}) = \hat{f}_{D_3}(3) = 7 \\
\hat{y}_{\text{new},4} &= \hat{f}_{D_4}(x_{\text{new}}) = \hat{f}_{D_4}(3) = 8
\end{aligned}
$$

- What is the bias and variance based on these models?

Numerical Example of Bias and Variance Tradeoff III

- Average prediction

$$\hat{f}_{\text{avg}}(x_{\text{new}}) = \hat{f}_{\text{avg}}(3) = \frac{1}{4}(6+7+7+8) = 7.$$

- Bias

$$\text{Bias} = \hat{f}_{\text{avg}}(x_{\text{new}}) - f(x_{\text{new}}) = \hat{f}_{\text{avg}}(x_{\text{new}}) - y_{\text{new}} = 7 - 7.5 = -\frac{1}{2}.$$

- Variance

$$\begin{aligned} \text{Variance} &= E_D\left[\left(\hat{f}_{\text{avg}}(x_{\text{new}}) - \hat{f}_D(x_{\text{new}})\right)^2\right] \\ &= \frac{1}{4}\left((6-7)^2 + (7-7)^2 + (7-7)^2 + (8-7)^2\right)^2 = \frac{1}{2} \end{aligned}$$

Numerical Example of Bias and Variance Tradeoff IV

- If there is no irreducible noise, using the bias-variance formula,

$$\mathrm{MSE} = \mathrm{Bias}^2 + \mathrm{Variance} = \left(-\frac{1}{2}\right)^2 + \frac{1}{2} = \frac{3}{4}.$$

- Now, using actual definition of MSE

$$\begin{aligned}
\mathrm{MSE} &= E_D\left[\left(\hat{f}_D(x_{\mathrm{new}}) - f(x_{\mathrm{new}})\right)^2\right] \\
&= \frac{1}{4}\left((6-7.5)^2 + (7-7.5)^2 + (7-7.5)^2 + (8-7.5)^2\right)^{\cancel{2}} \\
&= \frac{3}{4}
\end{aligned}$$

- Voila!

Bias-Variance Python Demo

```
import numpy as np
from sklearn.model_selection import train_test_split
from sklearn.linear_model import LinearRegression, Ridge
from sklearn import datasets
```

```
# preparing the dataset into inputs (feature matrix) and outputs (target vector)
data = datasets.load_boston()  # fetch the data
X = data.data  # feature matrix
y = data.target  # target vector

# split the data into training and test samples
X_train, X_test, y_train, y_test = train_test_split(X, y, test_size=0.3)
```

- Here, we are loading the Boston Housing dataset
- We split the raw dataset into 70% training and 30% testing in the last line
- Use .shape to check the dimensions of the various matrices!
- X_train.shape should give (354,13)

Bias-Variance Python Demo

```
def draw_bootstrap_sample(rng, X, y):
    sample_indices = np.arange(X.shape[0])
    bootstrap_indices = rng.choice(
        sample_indices, size=sample_indices.shape[0], replace=True
    )
    return X[bootstrap_indices], y[bootstrap_indices]
```

- Here, we are drawing various datasets from the given training set
- We are using a technique known as bootstrapping
- <u>**You don’t need to know this!**</u>
- This simulates the effect of …

$$\text{Think of } E_D \text{ as averaging across } \infty \text{ trials}$$

Bias-Variance Python Demo

```
def bias_variance_decomp(estimator, X_train, y_train, X_test, y_test, num_rounds=200, random_seed=20):
    rng = np.random.RandomState(random_seed)

    all_pred = []
    for i in range(num_rounds):
        # do bootstrap sampling, i.e., sampling with replacement
        X_boot, y_boot = draw_bootstrap_sample(rng, X_train, y_train)

        # fit a model on bootstrap samples and make prediction on test samples
        pred = estimator.fit(X_boot, y_boot).predict(X_test)
        all_pred.append(pred)

    all_pred = np.array(all_pred)

    # calculate MSE
    avg_mse = ((all_pred - y_test[None,:])**2).mean() # y_test[None,:] will reshape y_test from (N,) to (1,N)

    # average prediction of all bootstrap models on test set
    avg_predictions = np.mean(all_pred, axis=0)

    # calculate bias squared
    avg_bias = np.sum((avg_predictions - y_test) ** 2) / y_test.size

    # calculate variance
    avg_var = np.sum((avg_predictions - all_pred) ** 2) / all_pred.size

    return avg_mse, avg_bias, avg_var
```

$$E_D\left[\left(y(x)-\hat{f}_D(x)\right)^2\right]$$

$$\mathrm{Bias}(\hat{f})=\hat{f}_{avg}(x)-f(x),$$

$$\mathrm{Var}(\hat{f})=E_D\left[\left(\hat{f}_D(x)-\hat{f}_{avg}(x)\right)^2\right]$$

- The different samples of the training dataset D are collected in all_pred
- The mean-squared error is calculated in avg_mse
- The bias squared is calculated in avg_bias
- The variance is calculated in avg_var

Bias-Variance Python Demo

```
# define the model
model = LinearRegression()

# estimating the bias and variance
avg_mse, avg_bias, avg_var = bias_variance_decomp(model, X_train,
                                                  y_train, X_test,
                                                  y_test,
                                                  num_rounds=500,
                                                  random_seed=0)

# summary of the results
print('Average mean-squared error: %.3f' % avg_mse)
print('Average bias: %.3f' % avg_bias)
print('Average variance: %.3f' % avg_var)
```

```
Average mean-squared error: 27.360
Average bias: 26.064
Average variance: 1.296
```

- Here, we train a linear regression model.
- The MSE is indeed the squared bias plus the variance. Proof by python!
- There is no residual noise in this model.

Bias-Variance Python Demo

```
# define the model
model = Ridge(alpha=1)

# estimating the bias and variance
avg_mse, avg_bias, avg_var = bias_variance_decomp(model, X_train,
                                                  y_train, X_test,
                                                  y_test,
                                                  num_rounds=500,
                                                  random_seed=0)

# summary of the results
print('Average mean-squared error: %.3f' % avg_mse)
print('Average bias: %.3f' % avg_bias)
print('Average variance: %.3f' % avg_var)
model.coef_
```

```
Average mean-squared error: 27.375
Average bias: 26.133
Average variance: 1.242
```

- Here, we train a ridge regression model with lambda = 1.0 (it is alpha in python)
- Bias goes up, variance goes down as expected.
- MSE may go up or down.
- Try experimenting with different alpha's (or lambda's)!