

Bias-Variance trade-off for Model Selection

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#### Problem Statement

Take a trigonometric function and a choose an error function (N(0, sigma-sq)). Generate data set of 10,000 instances. Fit polynomials of order 1 - 10 and estimate and plot total error, Bias, Variance,

training and validation error for each using 10-fold cross validation. Create the folds using Python function and compute all errors using the equations given in textbook. Select the optimal model.

For the selected model, estimate and plot total error, Bias, Variance, training and validation error for training set sizes 1K, 2K, ... 10K. Use 10-fold cross validation for each training set, and the functions coded earlier for estimating the error.

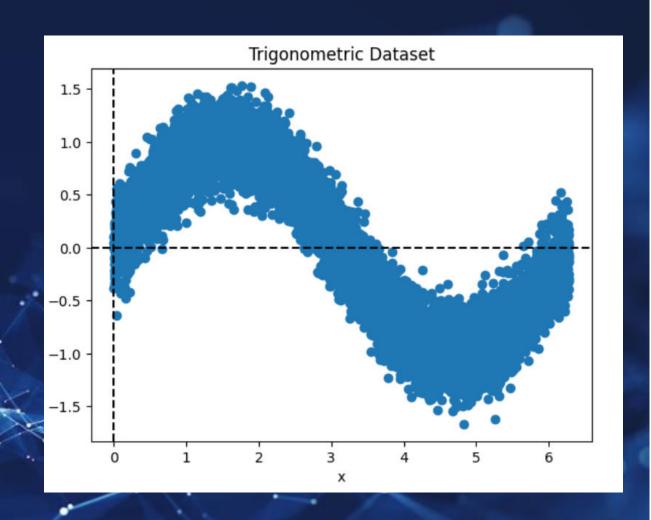
#### Dataset Generation

- Trignometric function is taken as user input using format np.trig\_func e.g. np.sin for sine.
- Angles are generated using random function and noise using normal distribution(randomly).
- Dataframe is generated from the dataset generated.

```
def generate dataset(num instances, sigma, trig func):
   dataset = []
   for in range(num instances):
       angle = np.random.uniform(0, 2 * np.pi) # Random angle between 0 and 2*pi
       error = np.random.normal(0, sigma) # Random error from a normal distribution
       value = trig func(angle) + error # Compute the value with the user-defined trigonometric function and error
       dataset.append([angle, value])
   return dataset
num instances = 10000
sigma = 0.2 # Adjust the value of sigma to control the spread of the errors
# Get the user's input for the trigonometric function
trig func input = input("Enter the trigonometric function (e.g., 'np.sin' for sine): ")
trig func = eval(trig func input) # Evaluate the user's input to obtain the function
dataset = generate dataset(num instances, sigma, trig func)
# Create a DataFrame from the dataset
df = pd.DataFrame(dataset, columns=['x', 'y'])
df.head()
```

### Dataset Representation

- Input trignometric function : np.sin(i.e. sine function).
- x-axis represents the angle between 0 and  $2\pi$ .
- y-axis represents value of trignometric function for the given angle.



#### Value Calculation

- Training and testing error is calculated using mean squared error between actual and predicted values of training and testing dataset.
- Mean Squared Error :  $\sum (y y_i)^2/n$
- Bias and variance is calculated testing data.
- Total error= bias +variance

```
def calculate values(dataset, train indices, test indices, degree):
    x train = dataset[train indices, 0]
   y train = dataset[train indices, 1]
    x test = dataset[test indices, 0]
   y test = dataset[test indices, 1]
    coefficients = np.polyfit(x train, y train, degree)
    y train pred = np.polyval(coefficients, x train)
   y test pred = np.polyval(coefficients, x test)
   train error = mean squared error(y train, y train pred)
   test error = mean_squared_error(y_test, y_test_pred)
    bias = np.mean((y test - np.mean(y test pred))**2)
    variance = np.var(y test pred)
   total error = (bias+variance)
    return train error, test error, bias, variance, total error
```

# Polynomial Fitting

- We need to calculate bias, variance, training error, testing error and total error using 10-fold cross validation.
- K-fold cross validation: K-Fold is validation technique in which we split the data into k-subsets and the holdout method is repeated k-times where each of the k subsets are used as test set and other k-1 subsets are used for the training purpose. Then the average error from all these k trials is computed.

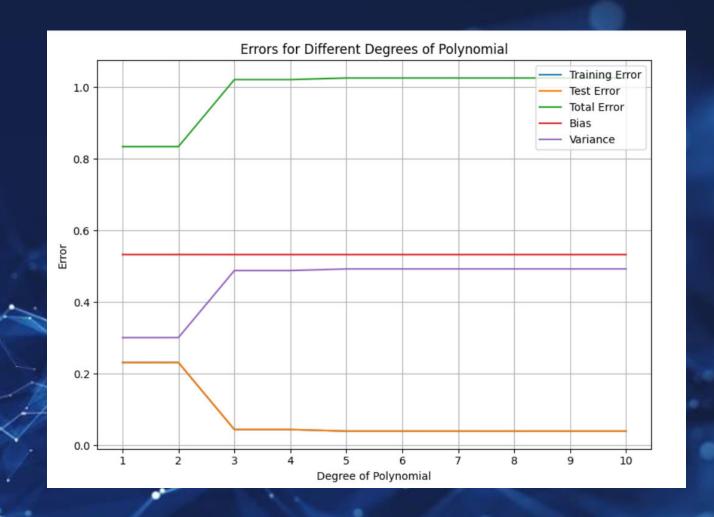
```
def fit polynomial(dataset, degrees, cv folds=10):
   kf = KFold(n_splits=cv_folds)
   total errors = []
   biases = []
   variances = []
   train errors = []
   test errors = []
   for d in degrees:
       total_errors.append([])
       biases.append([])
       variances.append([])
       train errors.append([])
       test errors.append([])
   for train indices, test indices in kf.split(dataset):
       for idx, degree in enumerate(degrees):
           train_error, test_error, bias, variance, total_error = calculate_values(dataset, train_indices, test_indices, degree)
           total errors[idx].append(total error)
           biases[idx].append(bias)
           variances[idx].append(variance)
           train_errors[idx].append(train_error)
           test errors[idx].append(test error)
   for idx in range(0, len(degrees)):
       total errors[idx] = np.mean(total errors[idx])
       biases[idx] = np.mean(biases[idx])
       variances[idx] = np.mean(variances[idx])
       train errors[idx] = np.mean(train errors[idx])
       test_errors[idx] = np.mean(test_errors[idx])
   return total_errors, biases, variances, train_errors, test_errors
```

#### Bias, Variance, Training Error, Testing Error and Total Error

Training Set Size	Total Error	Bias	Variance	Training Error	Testing Error	
1000	1.06137	0.551319	0.510056	0.0404971	0.0410599	
2000	1.05077	0.54495	0.505817	0.0382795	0.0385956	
3000	1.03895	0.539134	0.499813	0.0393754	0.0395735	
4000	1.04276	0.541245	0.501511	0.0397937	0.0399523	
5000	1.0469	0.543395	0.503509	0.0399773	0.0400813	
6000	1.04431	0.542235	0.502071	0.0398689	0.0399881	
7000	1.03702	0.538437	0.498581	0.0397866	0.0398784	
8000	1.03994	0.539881	0.500062	0.0398606	0.0399548	
9000	1.03823	0.539036	0.49919	0.0398423	0.0399195	
10000	1.03281	0.53637	0.496444	0.0400131	0.0400757	

# Error Plotting

- Bias, Variance, Training error, Testing error and Total error generated earlier is plotted for different degree of polynomial.
- x-axis represents the degree of ploynomial.
- y-axis represents the error.



## Optimal degree Calculation

- Optimal degree is the degree of polynomial for which the model is best fit.
- For the taken function sin(in our case) the optimal degree is 7.

```
optimal_degree_idx = np.argmin(test_errors)
optimal_degree = degrees[optimal_degree_idx]
print(optimal_degree)
```

7

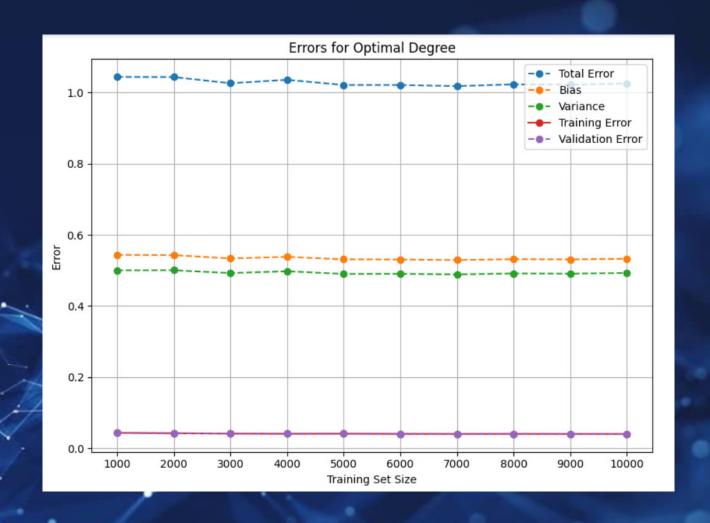
# Fitting Optimal Polynomial

- Till now optimal degree is calculated i.e. 7, now the optimal polynomial of degree 7 is needed to be fitted.
- Now the bias, variance, test error, training error and total error is calculated each for 1k,2k,3k,....,10k size dataset using 10-fold cross validation.

```
def fit optimal polynomial(dataset, degree, sizes):
    total errors = []
    biases = []
    variances = []
    train errors = []
    test errors = []
    for idx, size in enumerate(sizes):
        partial dataset = np.array(dataset[:size]) # Convert the dataset to a numpy array
        total error, bias, variance, train error, test error = fit polynomial(partial dataset, [degree])
        total errors.append(total error[0])
        biases.append(bias[0])
        variances.append(variance[0])
        train errors.append(train error[0])
        test errors.append(test error[0])
    return total errors, biases, variances, train errors, test errors
```

# Optimal Degree Error Plotting

- Finally the error plotting for the optimal degree i.e. 7(in our case) is done.
- x-axis shows Training set size i.e. 1k, 2k, 3k,....,10k.
- y-axis shows error.



## References

• Introduction to Machine Learning by Ethem Alpaydin.

# Thank You...