Deep Learning
Lab 5: Regularization

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Regularization

- Regularization refers to techniques that improve the generalizability of a trained model

Outline

- Scikit-learn
- Learning Theory
  - Error Curves and Model Complexity
  - Learning Curves and Sample Complexity
- Weight Decay
  - Ridge Regression
  - LASSO
- Validation
- Assignment

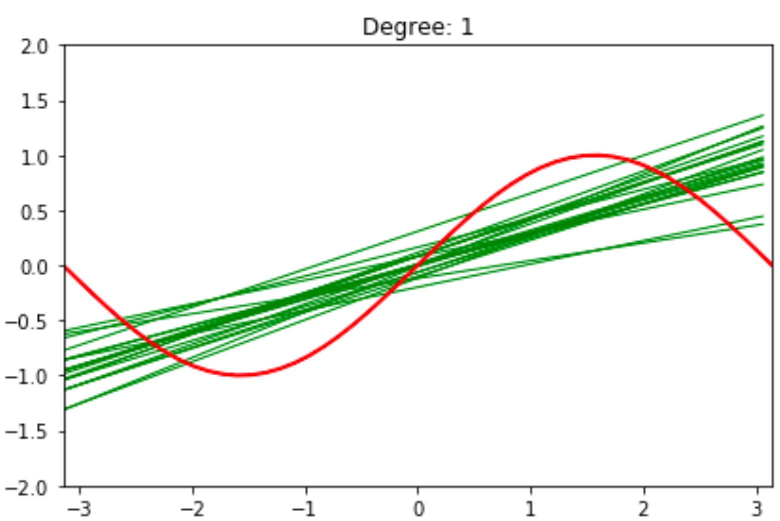
Scikit-learn

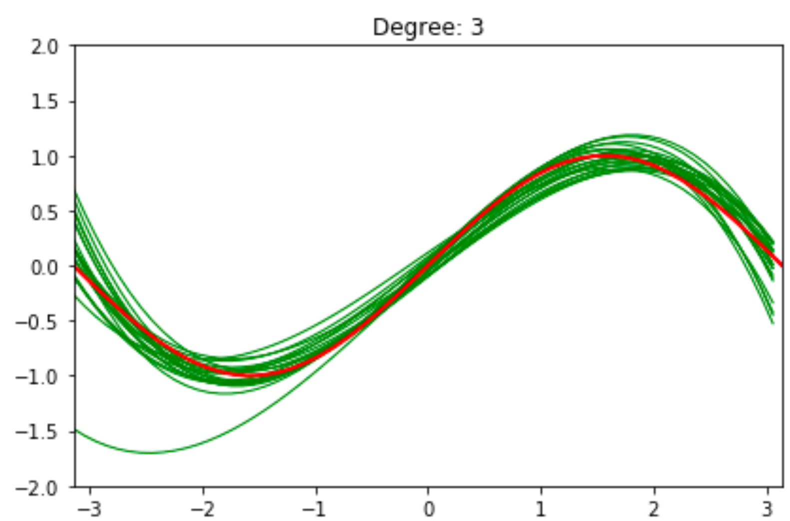
- Scikit-learn is a free software machine learning library for the Python programming language
- It features various classification, regression and clustering algorithms including support vector machines, random forests, gradient boosting, k-means and DBSCAN, and is designed to interoperate with the Python numerical and scientific libraries NumPy and SciPy
- pip install scikit-learn / conda install scikit-learn

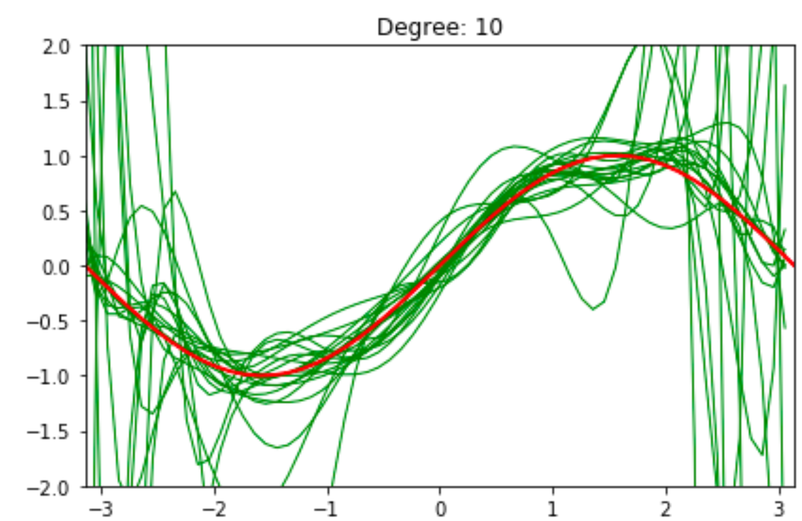
Learning Theory

- Learning theory provides a means to understand the generalizability of the model

- **Model complexity** plays a crucial role
  - Too simple: high bias and underfitting
  - Too complex: high variance and overfitting



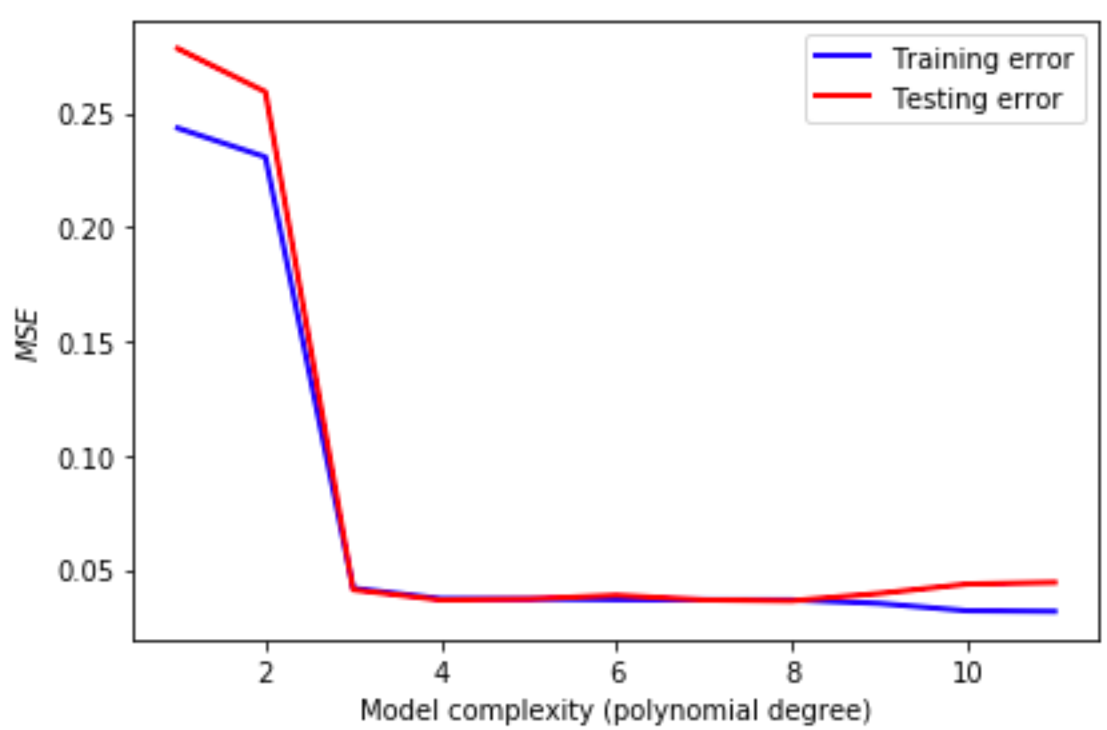




Error Curves and Model Complexity

- It is relatively hard to observe the figures showed in the last slide, since normally we will never know the data distribution of ground truth

- Instead, we can get those information by observing the training and testing error

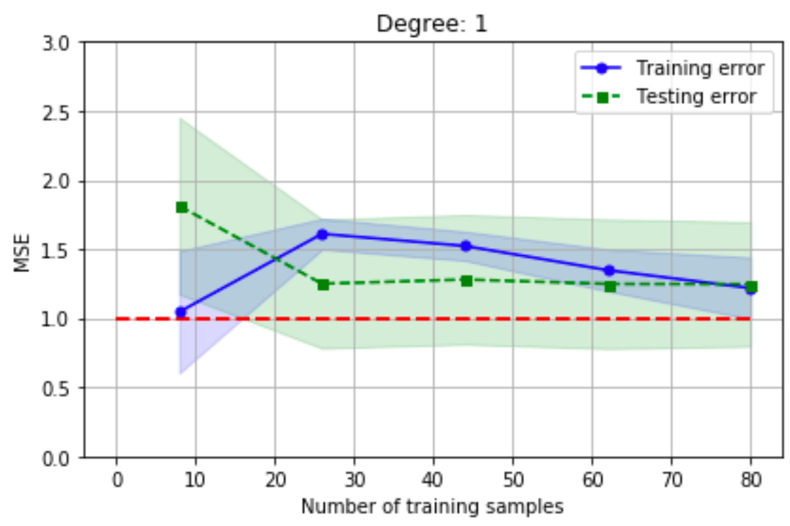


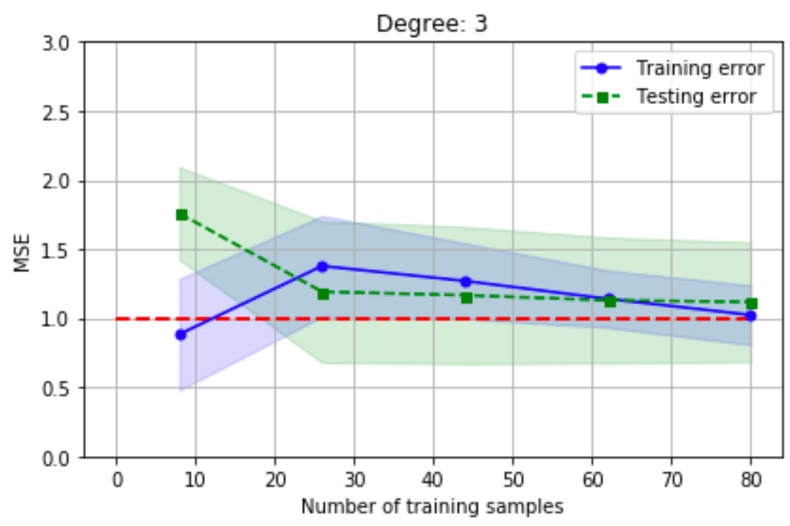
Error Curves and Model Complexity

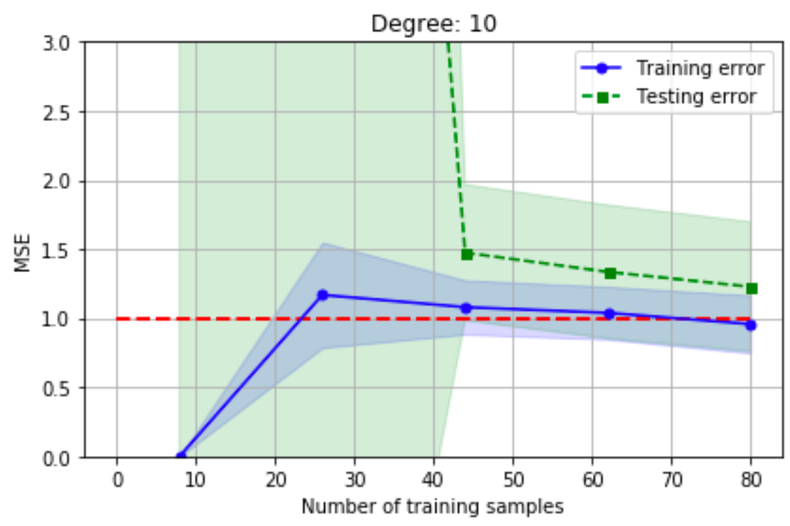
- Although the error curve visualizes the impact of model complexity, the bias-variance tradeoff holds only when you have sufficient training examples

Learning Curves and Sample Complexity

- The bounding methods of learning theory tell us that a model is likely to overfit regardless of it complexity **when the size of training set is small**. The **learning curves** are a useful tool for understanding how much training examples are sufficient







Weight Decay

- A common regularization approach. The idea is to add a term in the cost function against complexity
  - Ridge Regression (L_2)

$$\arg\min_{\boldsymbol{w},b} \|\boldsymbol{y} - (\boldsymbol{X}\boldsymbol{w} - b\mathbf{1})\|^2 + \alpha\|\boldsymbol{w}\|^2$$

  - LASSO (L_1)

$$\arg\min_{\boldsymbol{w},b} \|\boldsymbol{y} - (\boldsymbol{X}\boldsymbol{w} - b\mathbf{1})\|^2 + \alpha\|\boldsymbol{w}\|_1$$

Ridge Regression

- A small value α drastically reduces the testing error. Nevertheless, it's not a good idea to increase α forever, since it will over-shrink the coefficients of w and result in underfitting

$$\arg\min_{w,b} \|\boldsymbol{y} - (\boldsymbol{X}\boldsymbol{w} - b\mathbf{1})\|^2 + \alpha\|\boldsymbol{w}\|^2$$

```python
from sklearn.linear_model import Ridge
from sklearn.metrics import mean_squared_error

poly = PolynomialFeatures(degree=3)
X_poly = poly.fit_transform(X_std)
X_train, X_test, y_train, y_test = train_test_split(
    X_poly, y, test_size=0.3, random_state=0)

for a in [0, 1, 10, 100, 1000]:
    lr_rg = Ridge(alpha=a)
    lr_rg.fit(X_train, y_train)

    y_train_pred = lr_rg.predict(X_train)
    y_test_pred = lr_rg.predict(X_test)

    print('\n[Alpha = %d]' % a )
    print('MSE train: %.2f, test: %.2f' % (
                    mean_squared_error(y_train, y_train_pred),
                    mean_squared_error(y_test, y_test_pred)))
```

```
[Alpha = 0]
MSE train: 0.00, test: 19958.68

[Alpha = 1]
MSE train: 0.73, test: 23.05

[Alpha = 10]
MSE train: 1.66, test: 16.83

[Alpha = 100]
MSE train: 3.60, test: 15.16

[Alpha = 1000]
MSE train: 8.81, test: 19.22
```

LASSO

- An alternative weight decay approach that can lead to sparse w is the LASSO. Depending on the value of α, certain weights can become zero much faster than others

$$\arg\min_{\boldsymbol{w},b} \|\boldsymbol{y} - (\boldsymbol{X}\boldsymbol{w} - b\mathbf{1})\|^2 + \alpha\|\boldsymbol{w}\|_1$$

```
from sklearn.linear_model import Lasso
from sklearn.metrics import mean_squared_error

for a in [0.001, 0.01, 0.1, 1, 10]:
    lr_rg = Lasso(alpha=a)
    lr_rg.fit(X_train, y_train)

    y_train_pred = lr_rg.predict(X_train)
    y_test_pred = lr_rg.predict(X_test)

    print('\n[Alpha = %.2f]' % a )
    print('MSE train: %.2f, test: %.2f' % (
                mean_squared_error(y_train, y_train_pred),
                mean_squared_error(y_test, y_test_pred)))
```

```
[Alpha = 0.00]
MSE train: 19.96, test: 27.20

[Alpha = 0.01]
MSE train: 19.96, test: 27.28

[Alpha = 0.10]
MSE train: 20.42, test: 28.33

[Alpha = 1.00]
MSE train: 26.04, test: 33.41

[Alpha = 10.00]
MSE train: 84.76, test: 83.77
```

Ridge vs LASSO

- Why is LASSO sparse?
  - Ridge Regression (L_2)

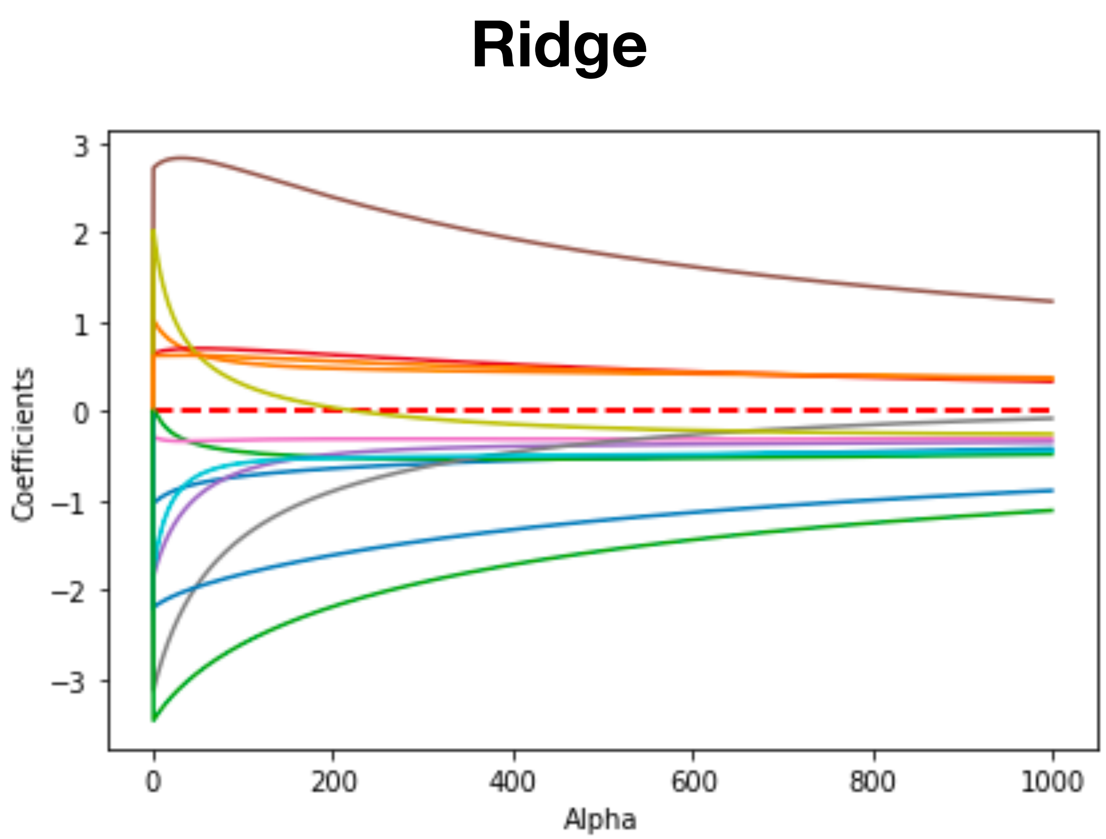
$$\arg\min_{\boldsymbol{w},b} \|\boldsymbol{y} - (\boldsymbol{X}\boldsymbol{w} - b\mathbf{1})\|^2 + \alpha\|\boldsymbol{w}\|^2$$

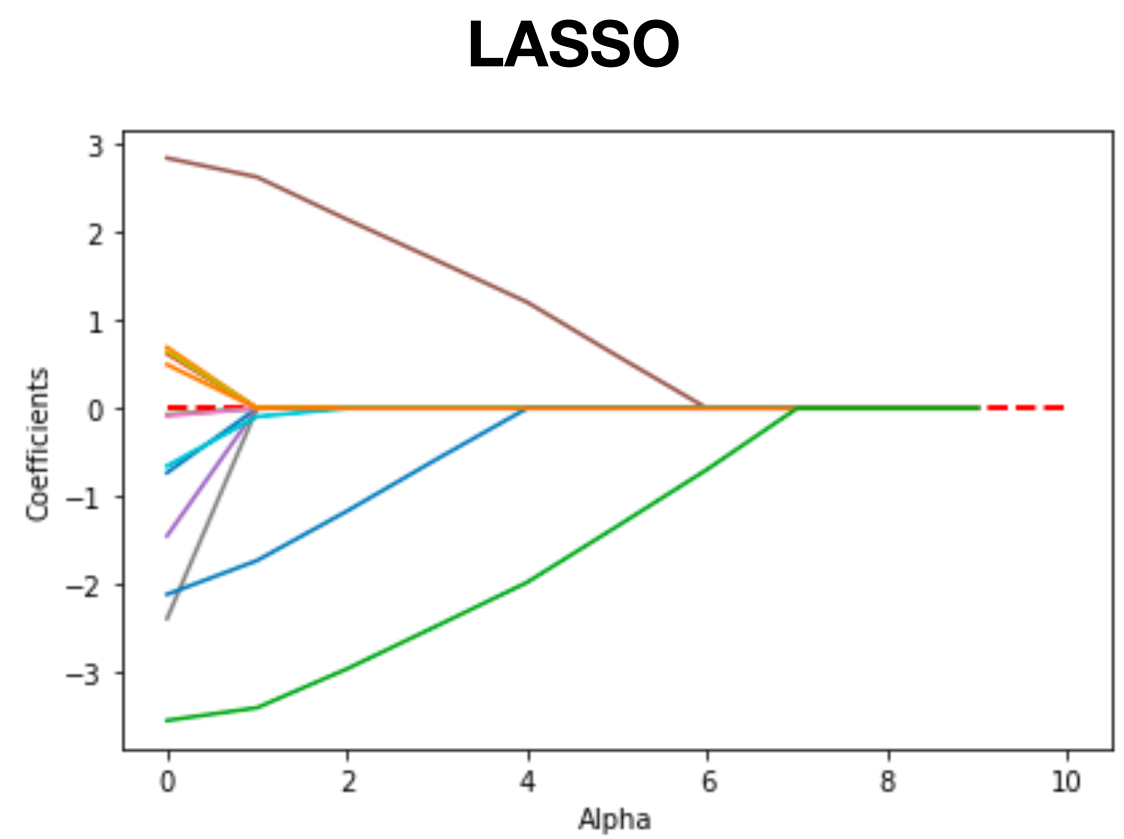
  - LASSO (L_1)

$$\arg\min_{\boldsymbol{w},b} \|\boldsymbol{y} - (\boldsymbol{X}\boldsymbol{w} - b\mathbf{1})\|^2 + \alpha\|\boldsymbol{w}\|_1$$

Initial weights		**Ridge Regression**
[1, 0.5, 1, 0.5]	►	**[0.5, 0.5, 0.5, 0.5]**
		LASSO
	►	**[0.5, 0, 0.5, 0]**

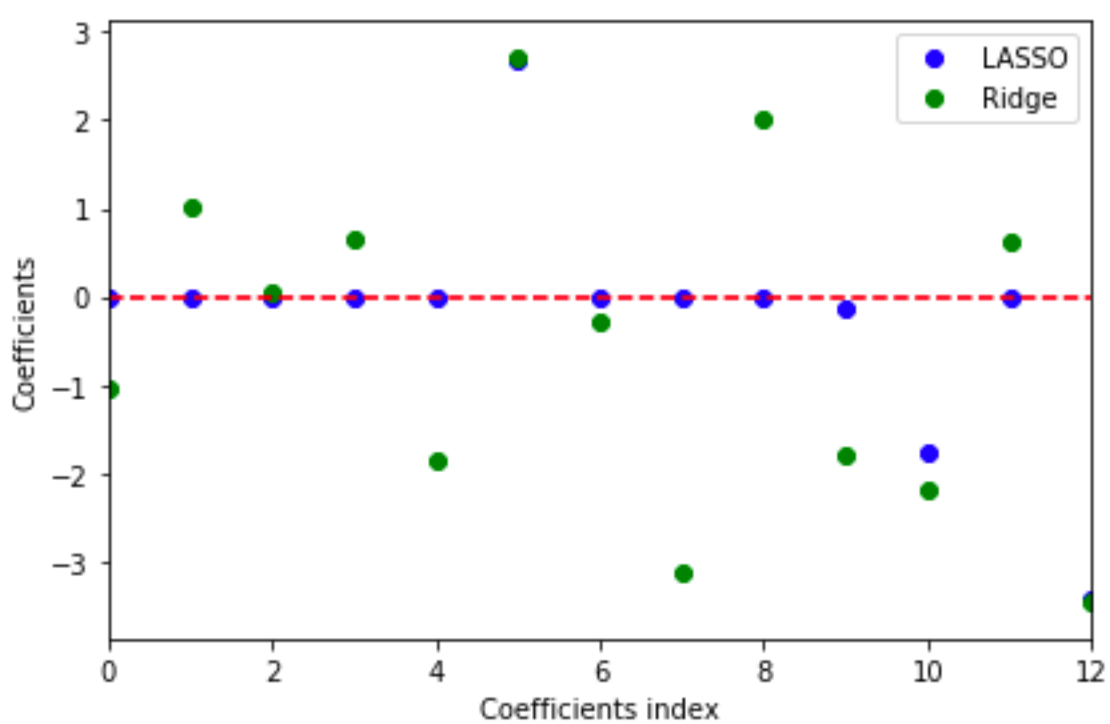
Ridge vs LASSO





Ridge vs LASSO

- LASSO can also be treated as a supervised feature selection technique when choosing a suitable regularization strength α to make only part of coefficients become exactly zeros

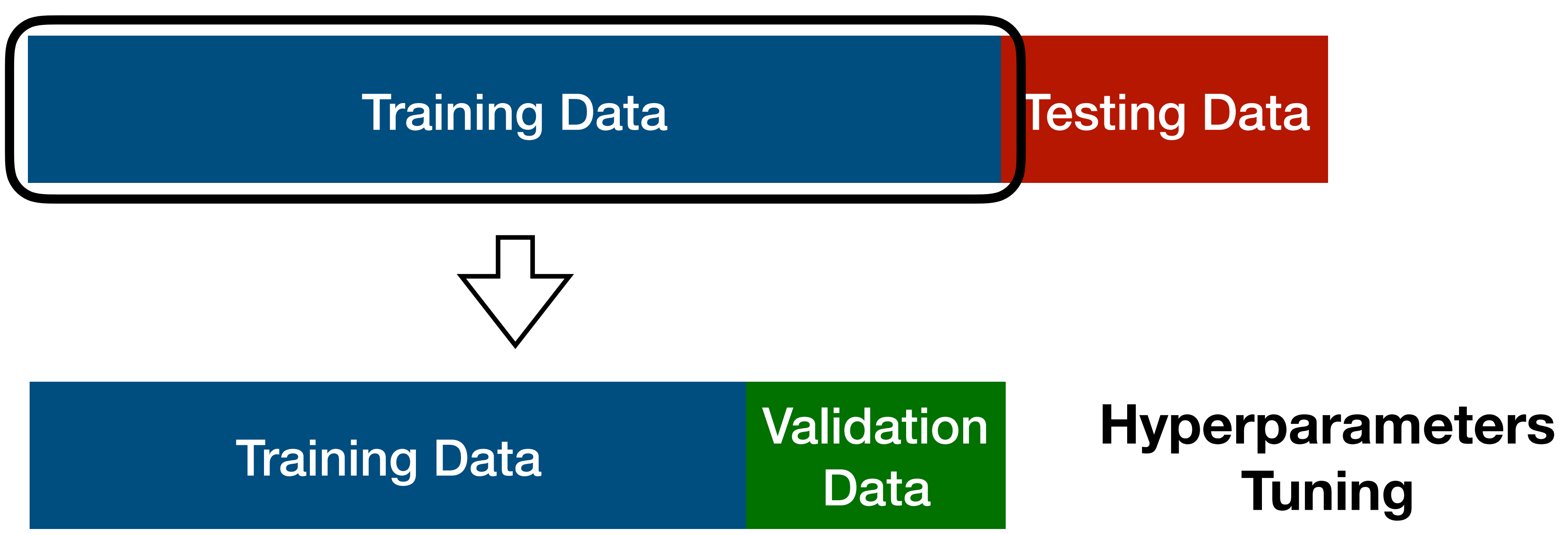


Validation

- Another useful regularization technique that helps us decide the proper value of hyperparameters

- The idea is to split your data into the training, validation, and testing sets and then select the best value based on validation performance

- NOTE: It is important that we should never peep testing data during training



Validation

```
[Degree = 1]
MSE train: 25.00, valid: 21.43, test: 32.09

[Degree = 2]
MSE train: 9.68, valid: 14.24, test: 20.24

[Degree = 3]
MSE train: 3.38, valid: 17.74, test: 18.63

[Degree = 4]
MSE train: 1.72, valid: 16.67, test: 30.98

[Degree = 5]
MSE train: 0.97, valid: 59.73, test: 57.02

[Degree = 6]
MSE train: 0.60, valid: 1444.08, test: 33189.41
```

Assignment

- In this assignment, you should train a model to predict if a shot can make under specific circumstance
  - **y_test** is hidden this time
  - Allow to use **any model** you have learned before to achieve the best accuracy
  - Select the best **3 features,** and show the accuracy with only those
- Hint
  - **Preprocess the data** to help your training
  - Since you don't have y_test this time, you may need to **split a validation set** for checking your performance

Assignment

- Submit to iLMS with
  your **ipynb** (Lab05_{student_id}.ipynb) and **y_pred.csv**

- The notebook should contain
  - How you **evaluate** your model
  - **All models** you have tried and the result
  - Plot the **error curve** of your best model and tell if it is **over-fit or not**
  - The top-3 features you find and how you find it
  - A **brief report** what you do in this assignment

- Deadline: 2019-10-03(Thur) 23:59