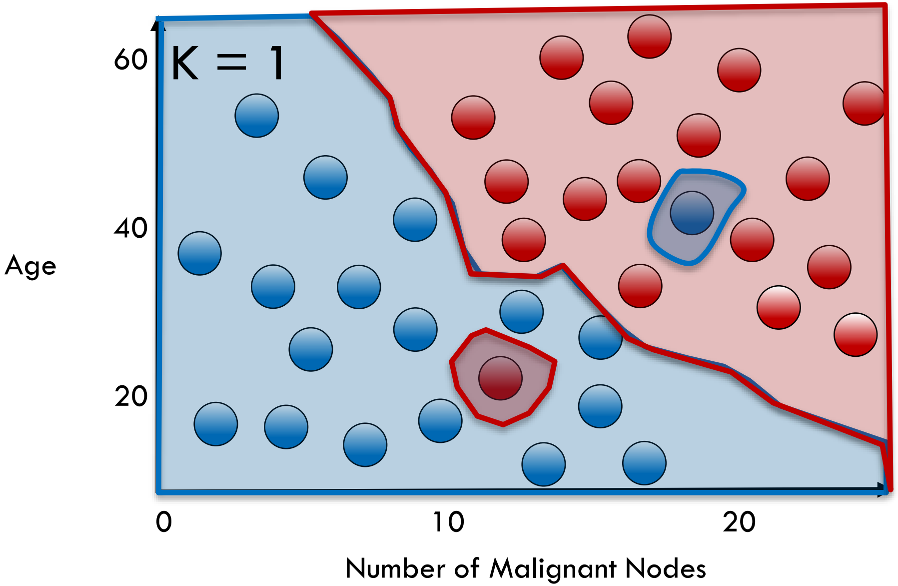
Model Generalization

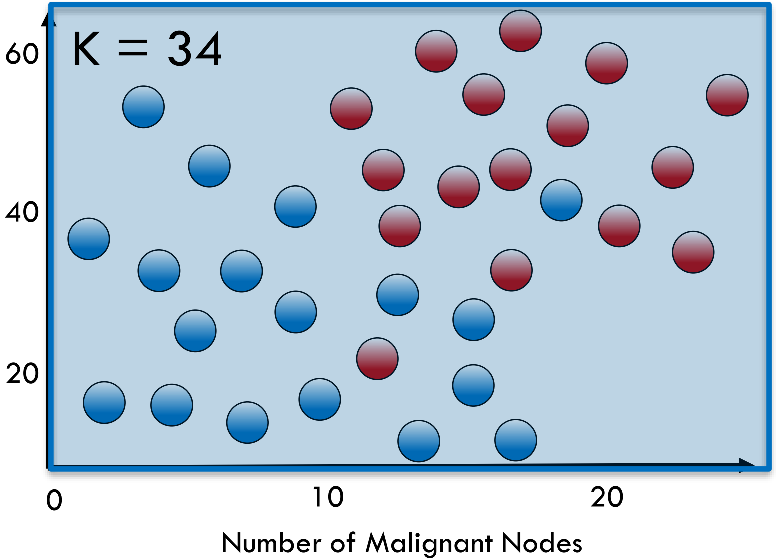
Legal Notices and Disclaimers

Learning Objectives

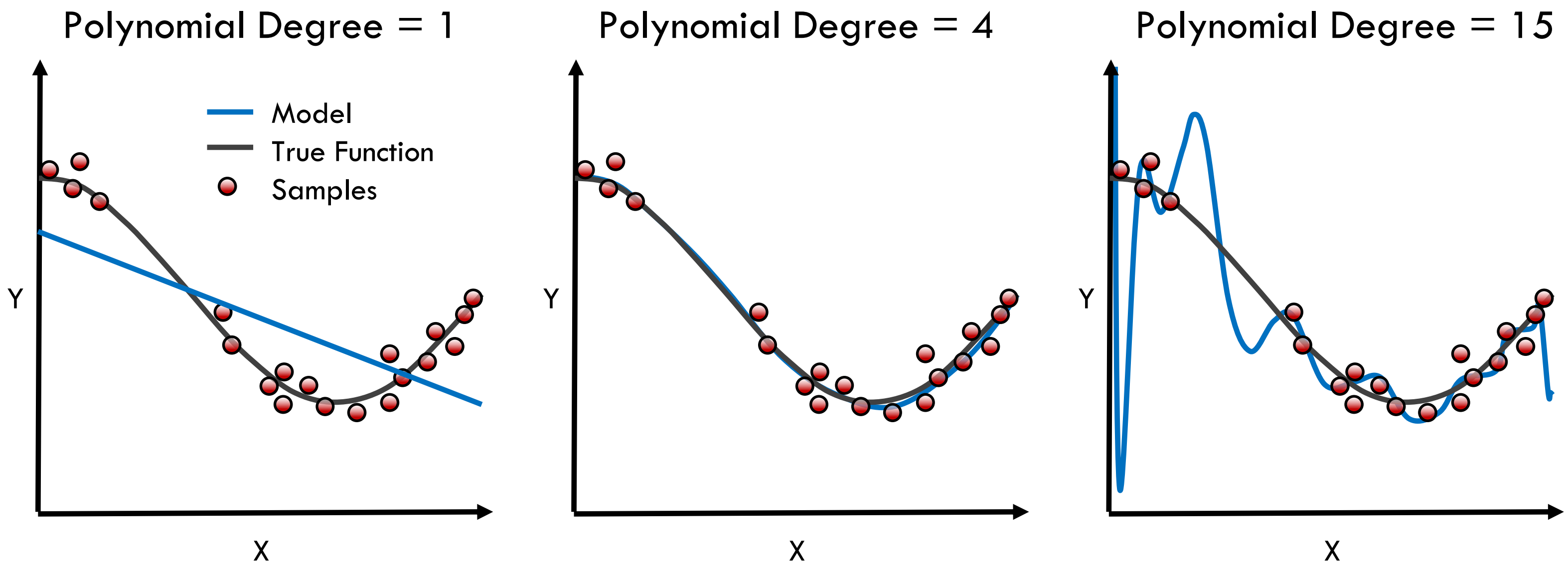
- Explain the difference between over-fitting and under-fitting a model
- Describe Bias-variance tradeoffs
- Find the optimal training and test data set splits, cross-validation, and model complexity versus error
- Apply a linear regression model for supervised learning
- Apply Intel® Extension for Scikit-learn* to leverage underlying compute capabilities of hardware

K Value Affects Decision Boundary

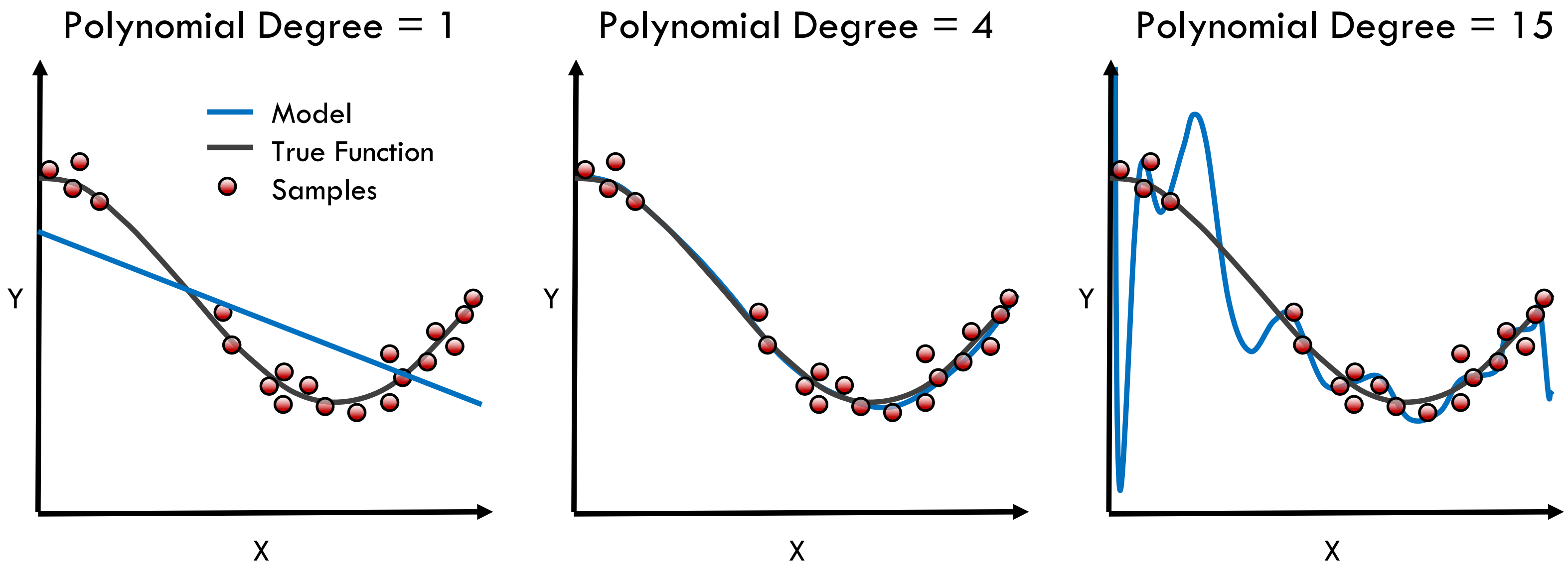




Choosing Between Different Complexities



How Well Does the Model Generalize?

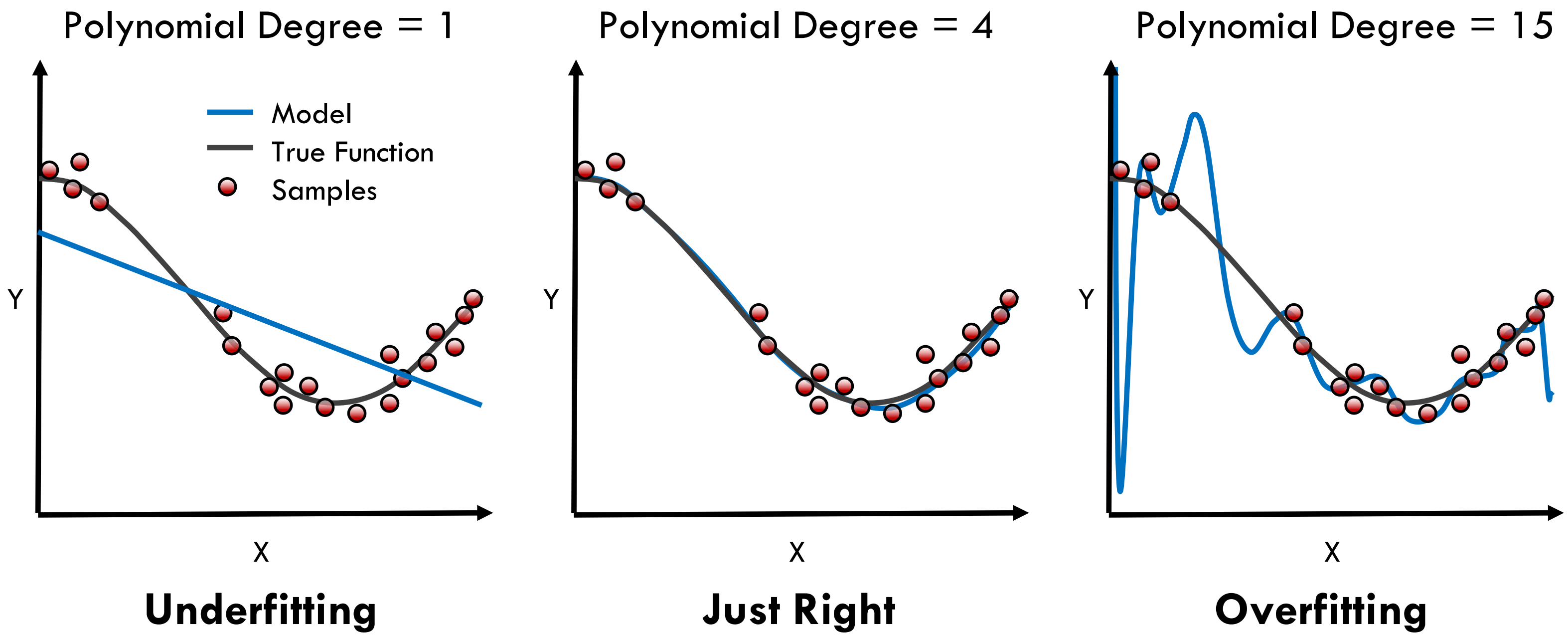


Poor at Training
Poor at Predicting

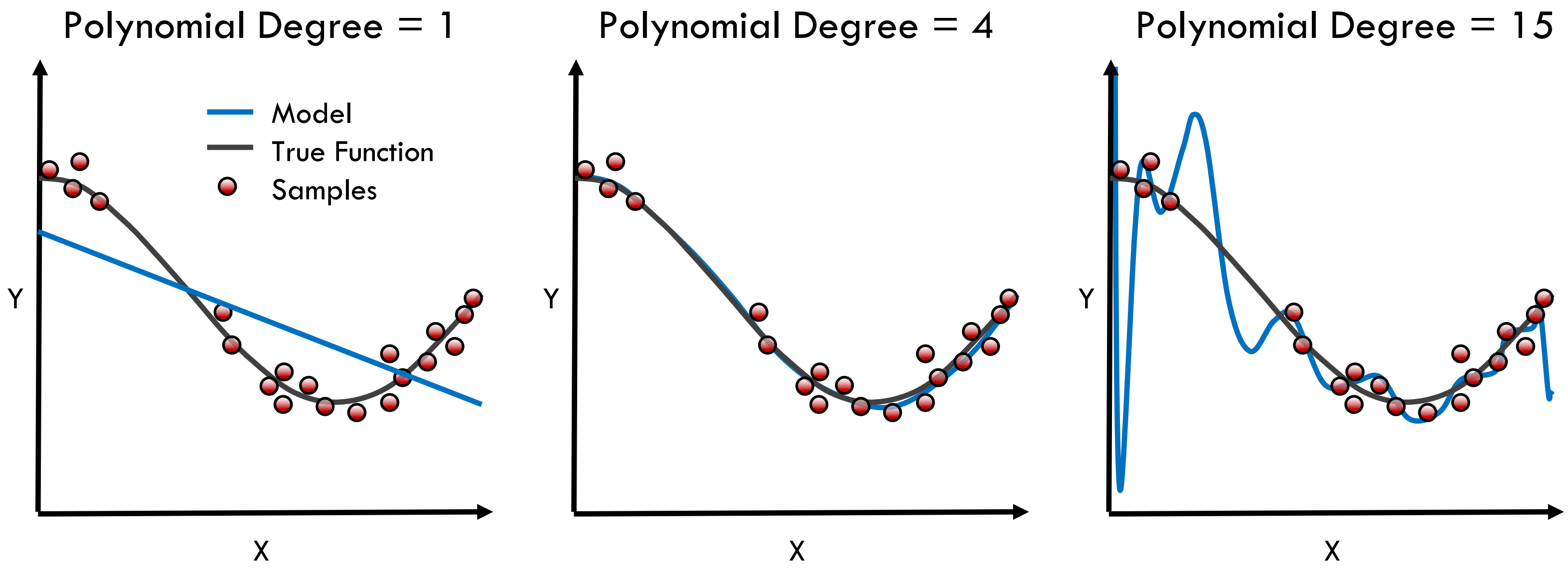
Just Right

Good at Training
Poor at Predicting

Underfitting vs Overfitting



Bias – Variance Tradeoff



High Bias
Low Variance

Just Right

Low Bias
High Variance

Training and Test Splits

	Date	Title	Budget	DomesticTotalGross	Director	Rating	Runtime
0	2013-11-22	The Hunger Games: Catching Fire	130000000	424668047	Francis Lawrence	PG-13	146
1	2013-05-03	Iron Man 3	200000000	409013994	Shane Black	PG-13	129
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7	2013-12-13	The Hobbit: The Desolation of Smaug	NaN	258366855	Peter Jackson	PG-13	161
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12	2013-06-21	World War Z	190000000	202359711	Marc Forster	PG-13	116
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15	2013-08-07	We're the Millers	37000000	150394119	Rawson Marshall Thurber	R	110
16	2013-12-13	American Hustle	40000000	150117807	David O. Russell	R	138
17	2013-05-10	The Great Gatsby	105000000	144840419	Baz Luhrmann	PG-13	143

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Training Data

Test Data

Using Training and Test Data

Training Data

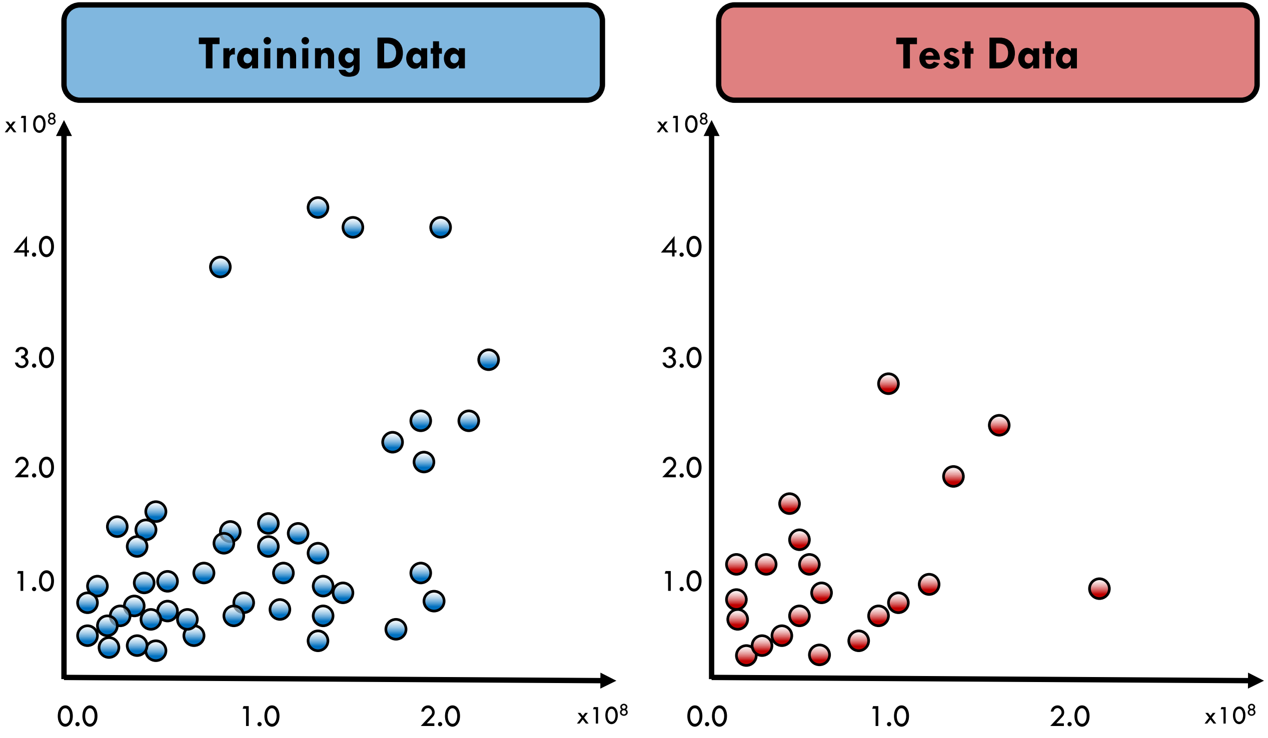
fit the model

Test Data

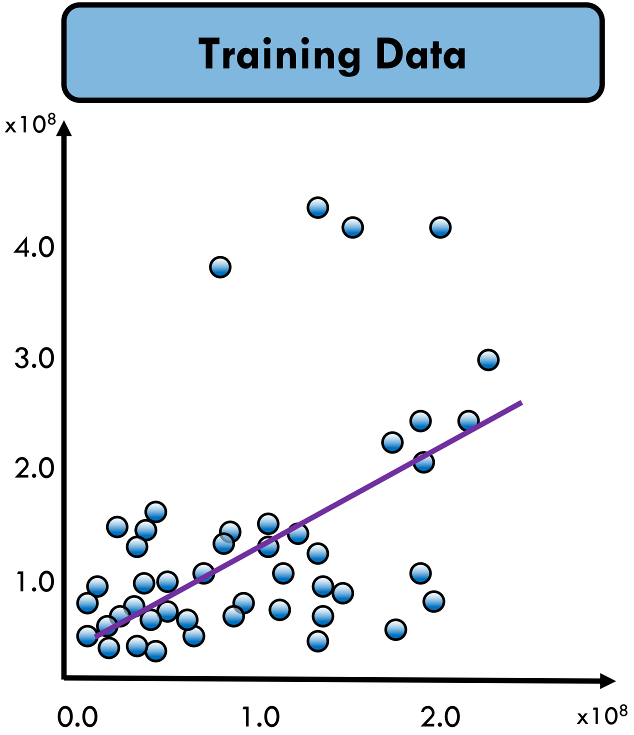
measure performance

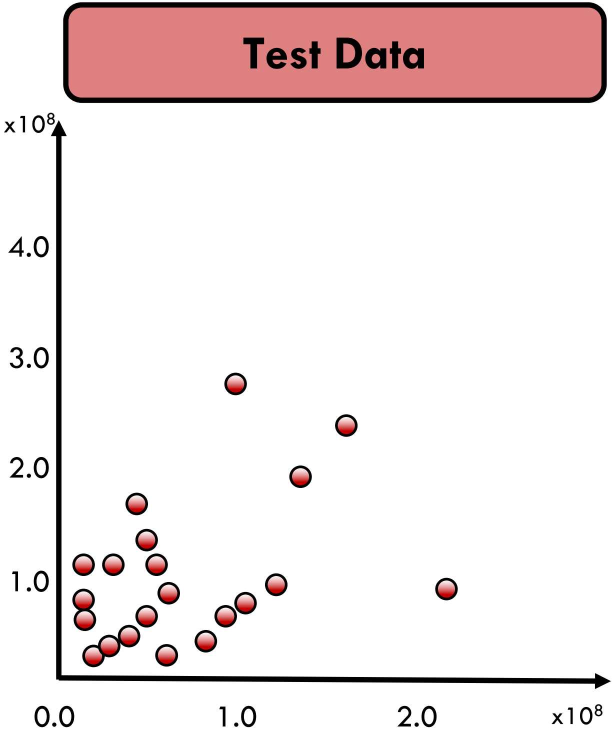
- predict label with model
- compare with actual value
- measure error

Using Training and Test Data



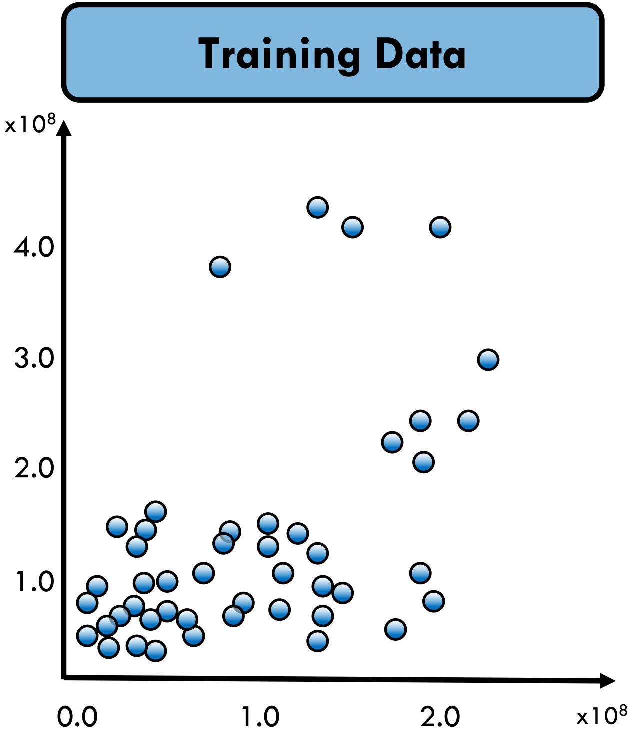
Using Training and Test Data

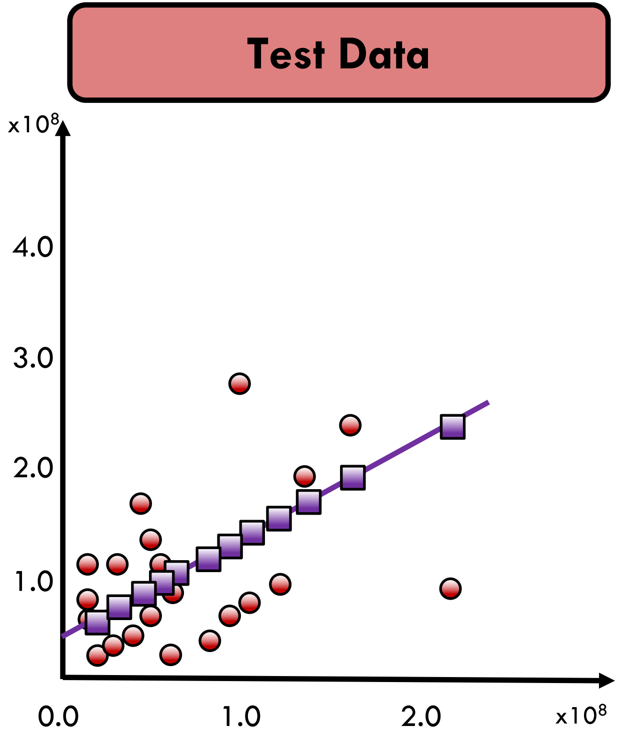




Fit the model

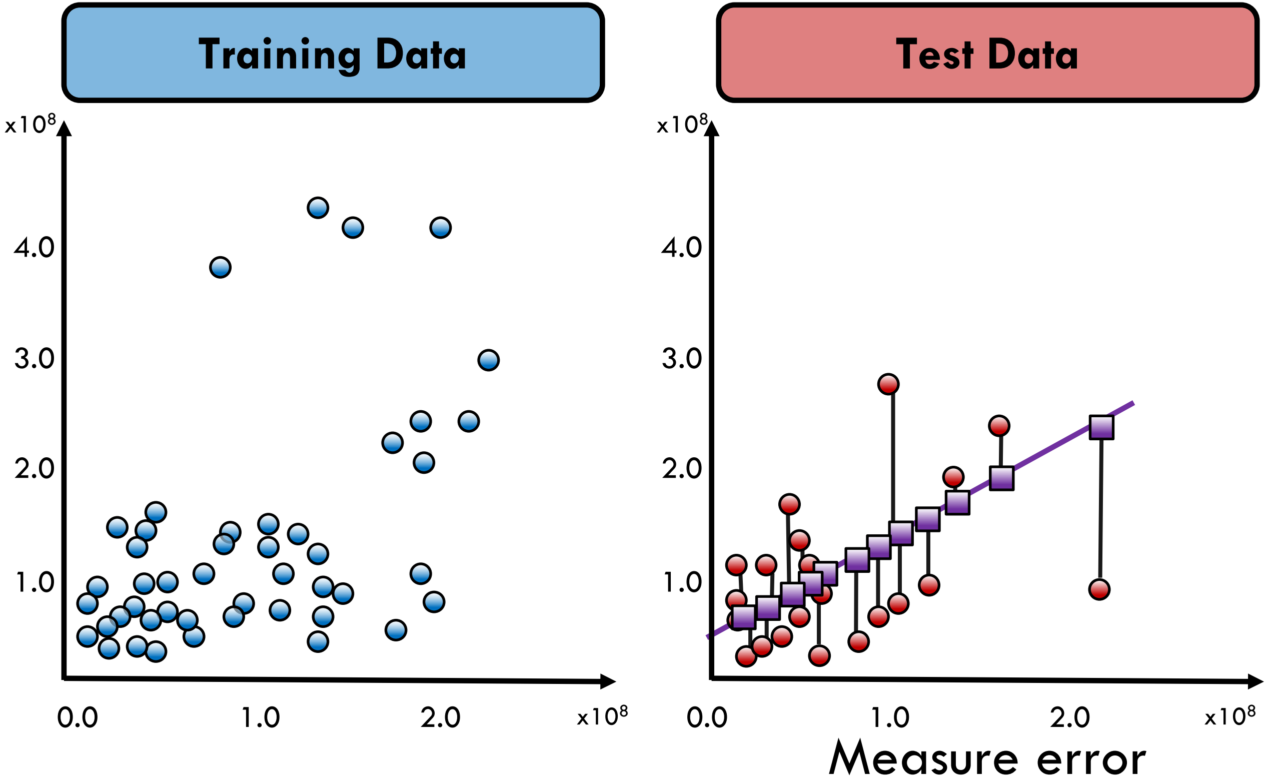
Using Training and Test Data



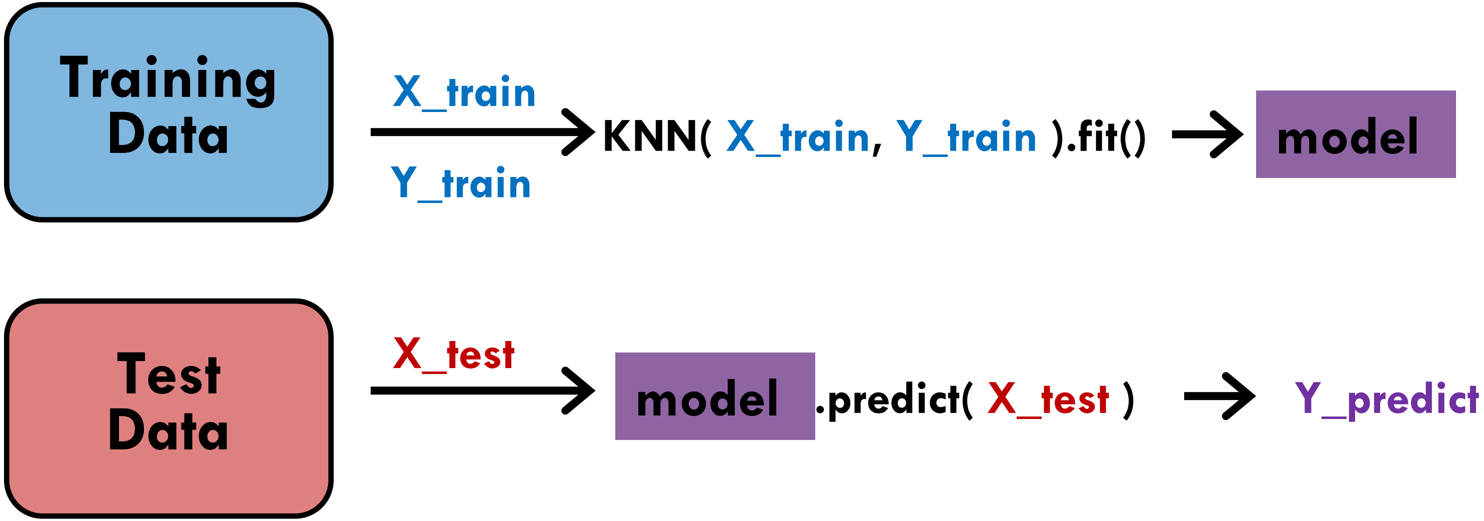


Make predictions

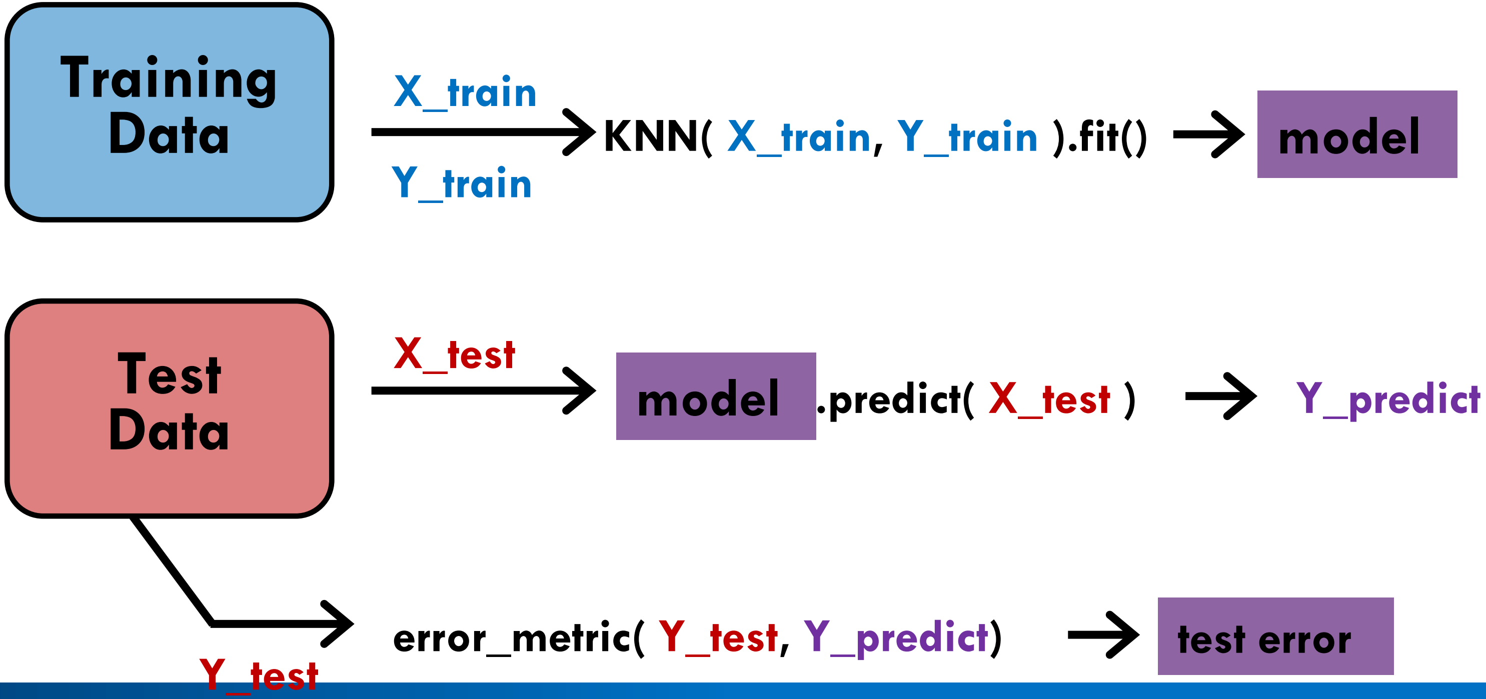
Using Training and Test Data



Fitting Training and Test Data



Fitting Training and Test Data



Train and Test Splitting: The Syntax

Import the train and test split function

```
from sklearn.model_selection import train_test_split
```

To use the Intel® Extension for Scikit-learn* variant of this algorithm:

- **Install Intel® oneAPI AI Analytics Toolkit (AI Kit)**
- **Add the following two lines of code before the above code:**

```
import patch_sklearn
patch_sklearn()
```

Train and Test Splitting: The Syntax

Import the train and test split function

```
from sklearn.model_selection import train_test_split
```

Train and Test Splitting: The Syntax

Import the train and test split function

```
from sklearn.model_selection import train_test_split
```

Split the data and put 30% into the test set

```
train, test = train_test_split(data, test_size=0.3)
```

Train and Test Splitting: The Syntax

Import the train and test split function

```
from sklearn.model_selection import train_test_split
```

Split the data and put 30% into the test set

```
train, test = train_test_split(data, test_size=0.3)
```

Other method for splitting data:

```
from sklearn.model_selection import ShuffleSplit
```

Beyond a Single Test Set: Cross Validation

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0	2013-11-22	The Hunger Games: Catching Fire	130000000	424668047	Francis Lawrence	PG-13	146
1	2013-05-03	Iron Man 3	200000000	409013994	Shane Black	PG-13	129
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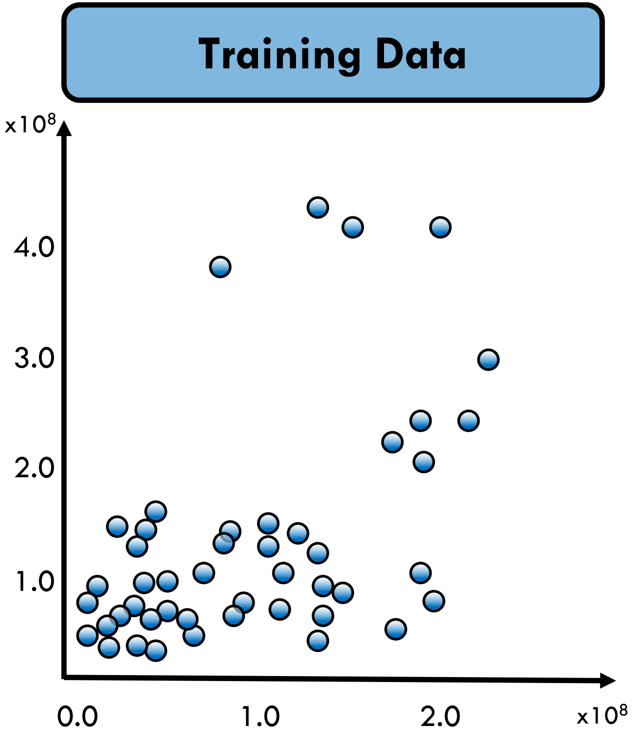
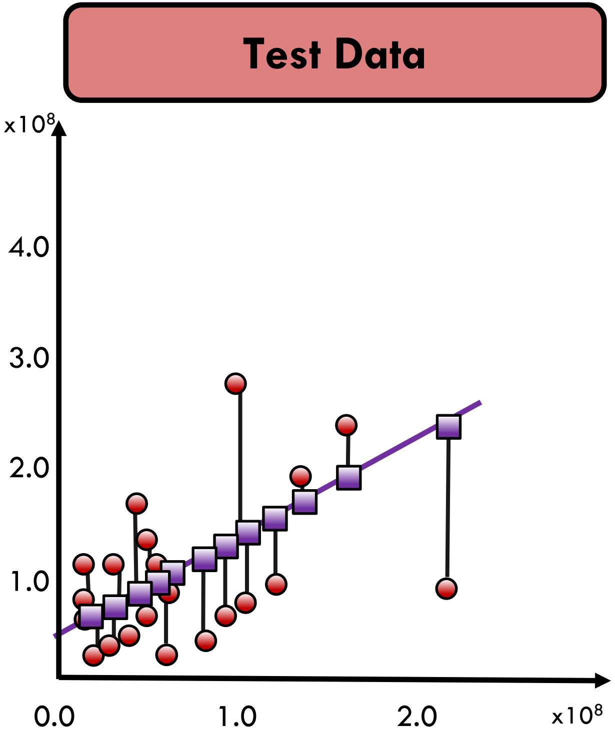
Training Data

Validation Data

Beyond a Single Test Set: Cross Validation





Best model for **<u>this</u>** test set

Beyond a Single Test Set: Cross Validation

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Training Data 1

Validation Data 1

Beyond a Single Test Set: Cross Validation

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Training Data 2

Validation Data 2

Beyond a Single Test Set: Cross Validation

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Validation Data 3

Training Data 3

Beyond a Single Test Set: Cross Validation

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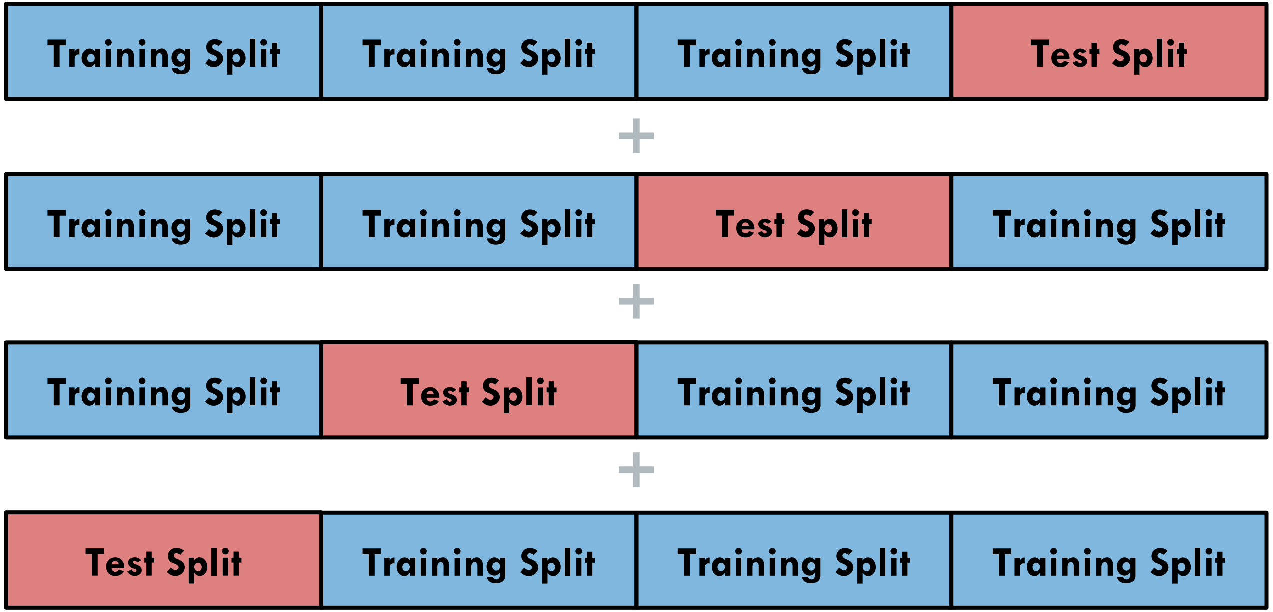
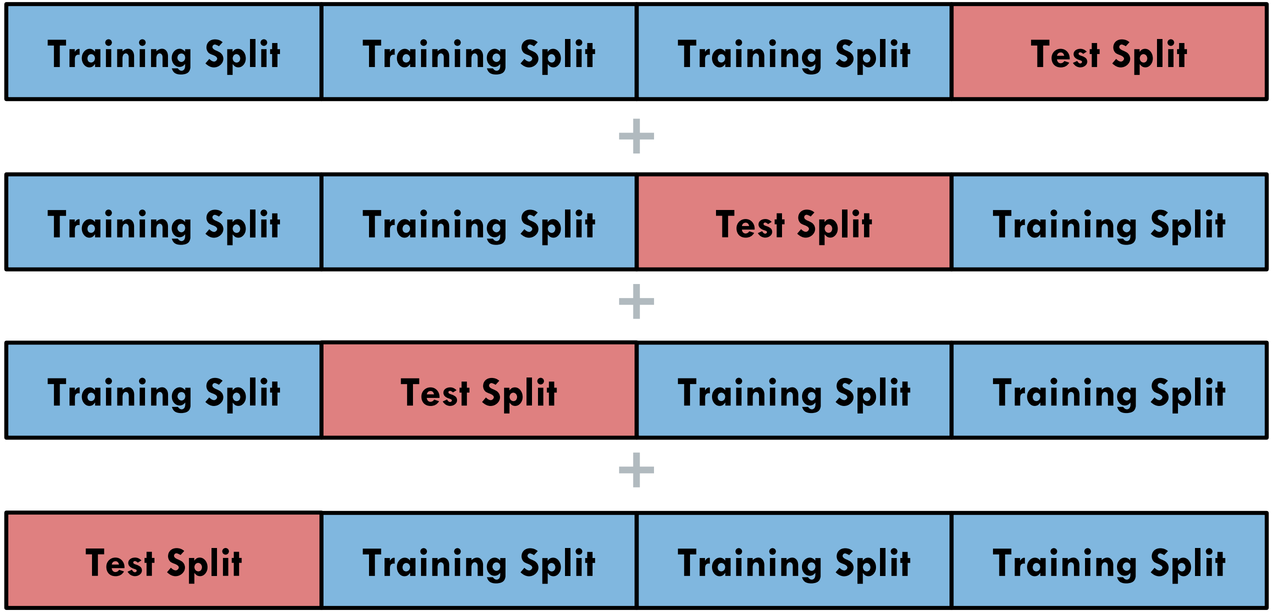
Validation Data 4

Training Data 4

Beyond a Single Test Set: Cross Validation

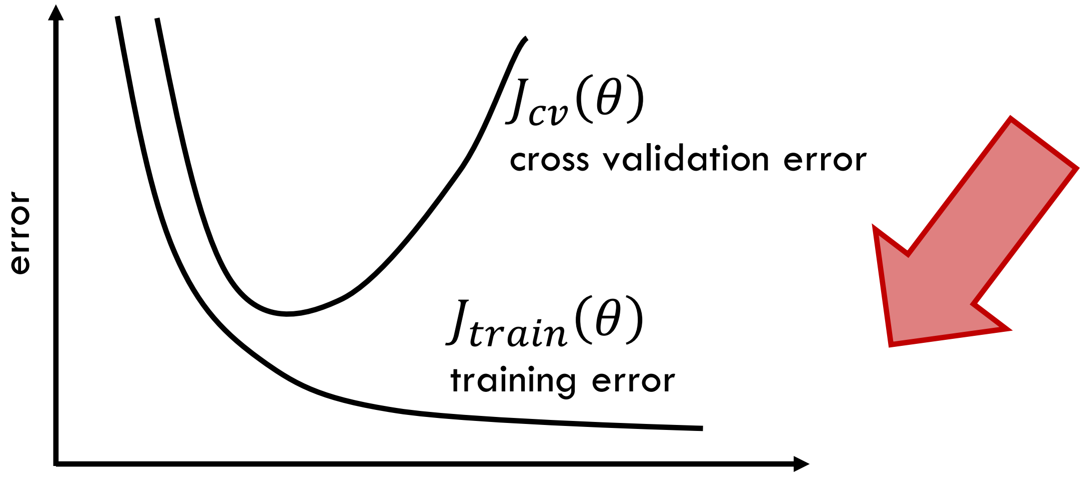


Beyond a Single Test Set: Cross Validation

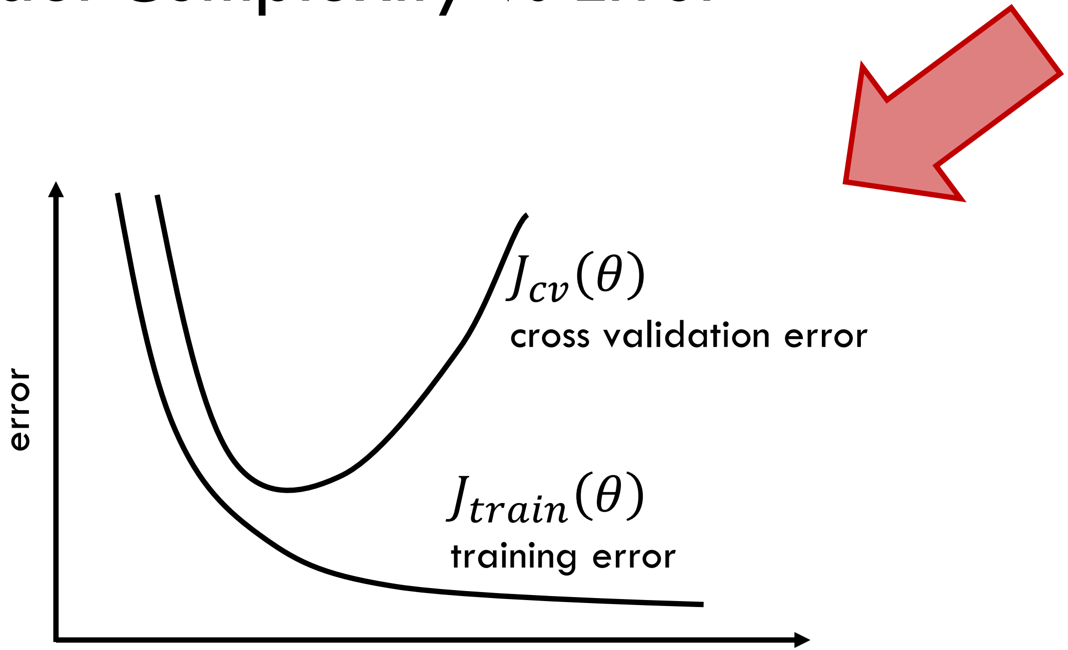


Average cross validation results.

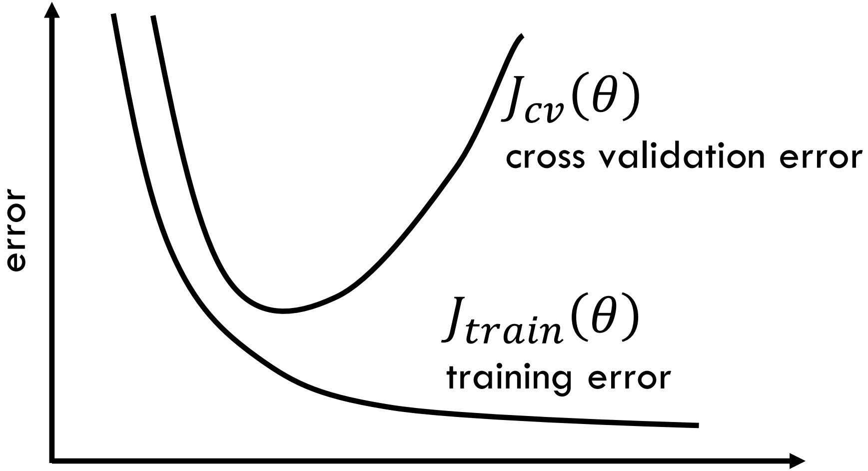
Model Complexity vs Error



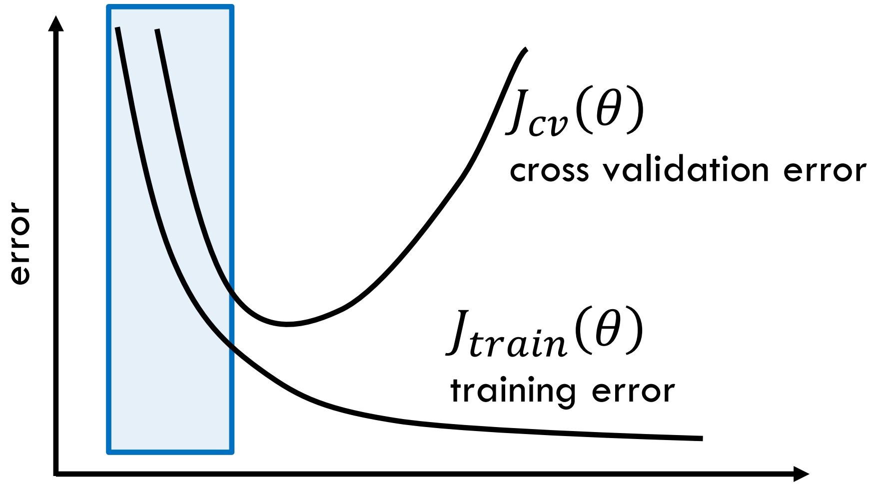
Model Complexity vs Error

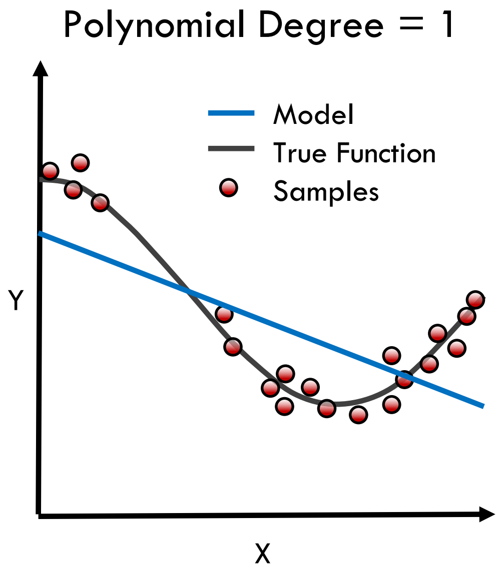


Model Complexity vs Error



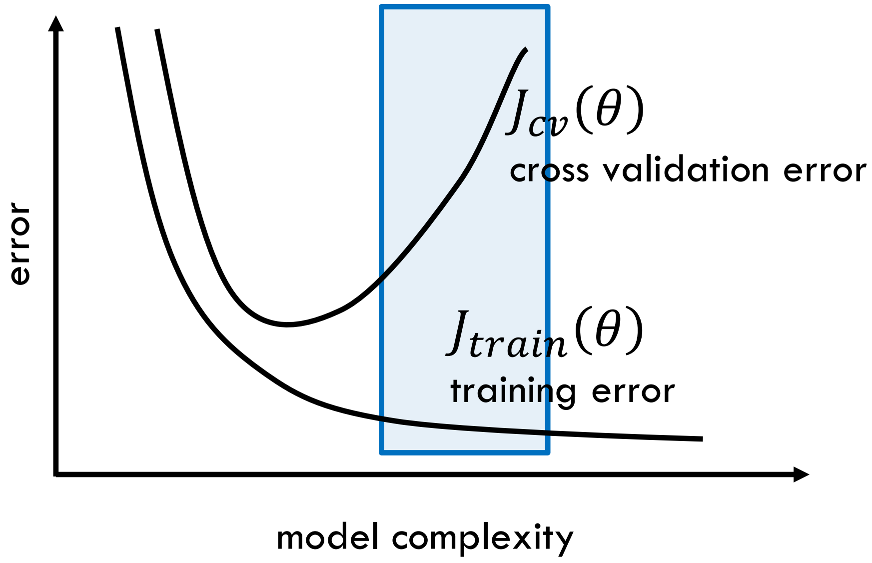
Model Complexity vs Error

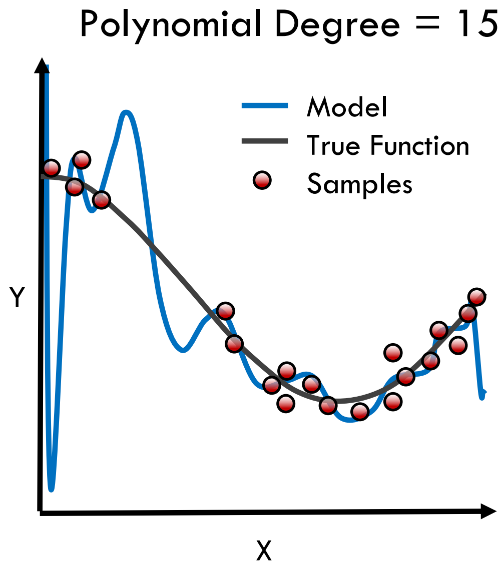




Underfitting: training and cross validation error are high

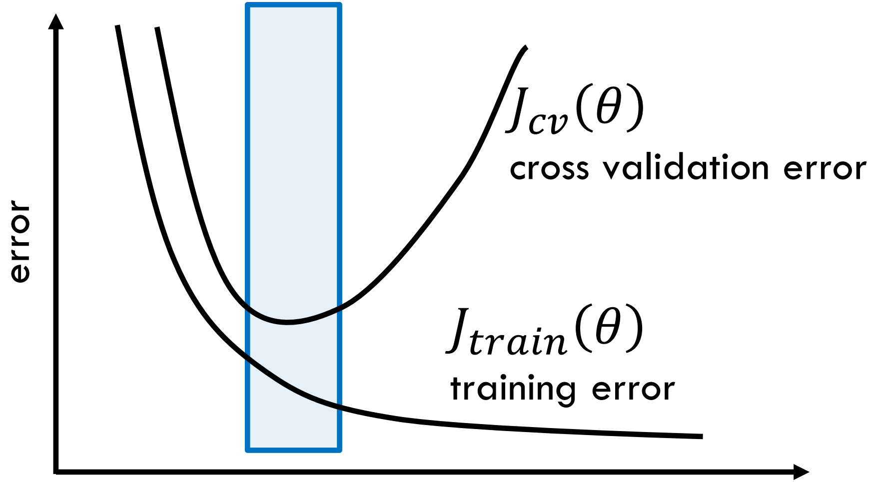
Model Complexity vs Error

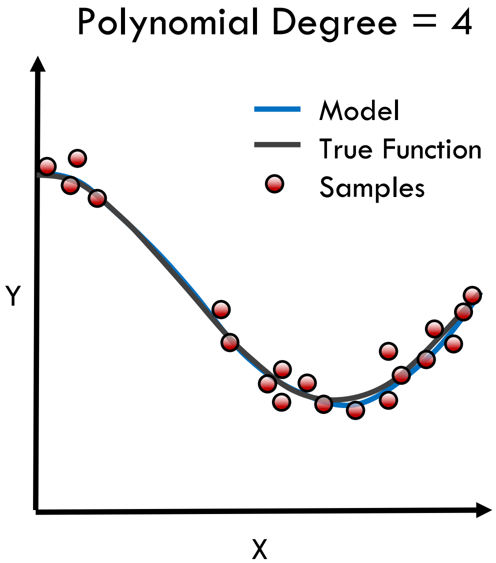




Overfitting: training error is low, cross validation is high

Model Complexity vs Error





Just right: training and cross validation errors are low

Cross Validation: The Syntax

Import the train and test split function

```
from sklearn.model_selection import cross_val_score
```

Cross Validation: The Syntax

Import the train and test split function

```
from sklearn.model_selection import cross_val_score
```

Perform cross-validation with a given model

```
cross_val = cross_val_score(KNN, X_data, y_data, cv=4,
            scoring='neg_mean_squared_error')
```

Cross Validation: The Syntax

Import the train and test split function

```
from sklearn.model_selection import cross_val_score
```

Perform cross-validation with a given model

```
cross_val = cross_val_score(KNN, X_data, y_data, cv=4,
                scoring='neg_mean_squared_error')
```

Other methods for cross validation:

```
from sklearn.model_selection import KFold, StratifiedKFold
```

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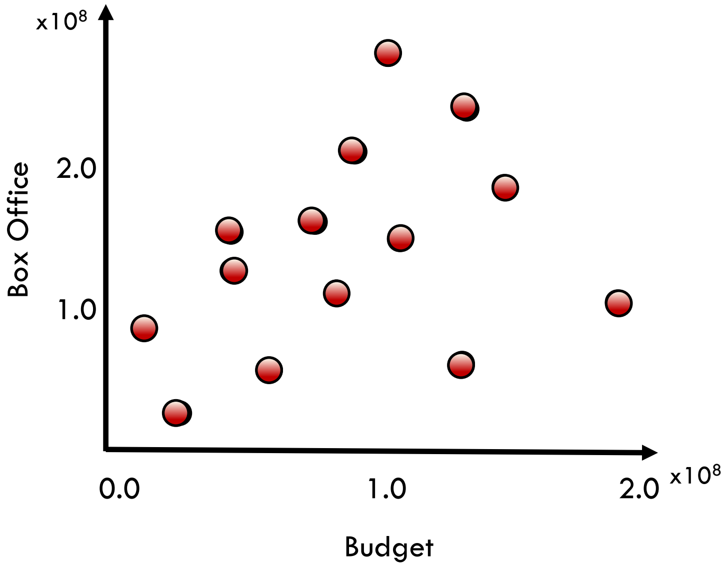
Software

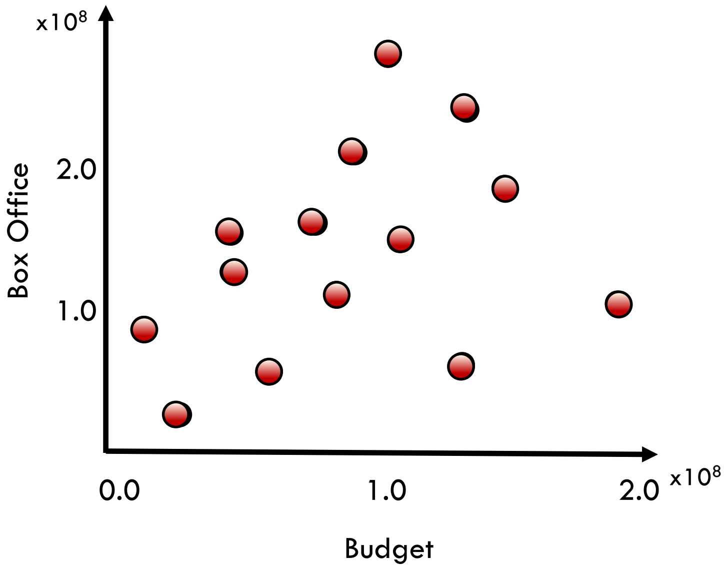
Introduction to Linear Regression

Introduction to Linear Regression



$$y_\beta(x) = \beta_0 + \beta_1 x$$

Introduction to Linear Regression



$$y_\beta(x) = \beta_0 + \beta_1 x$$

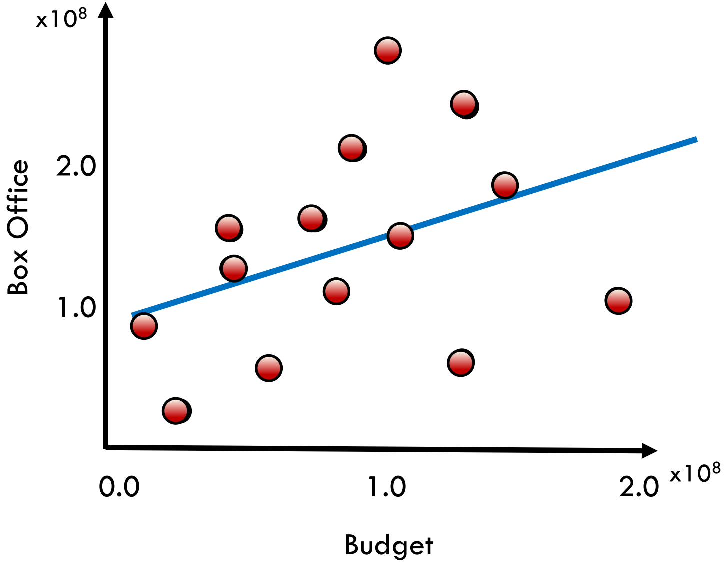
box office revenue

coefficient 0

coefficient 1

movie budget

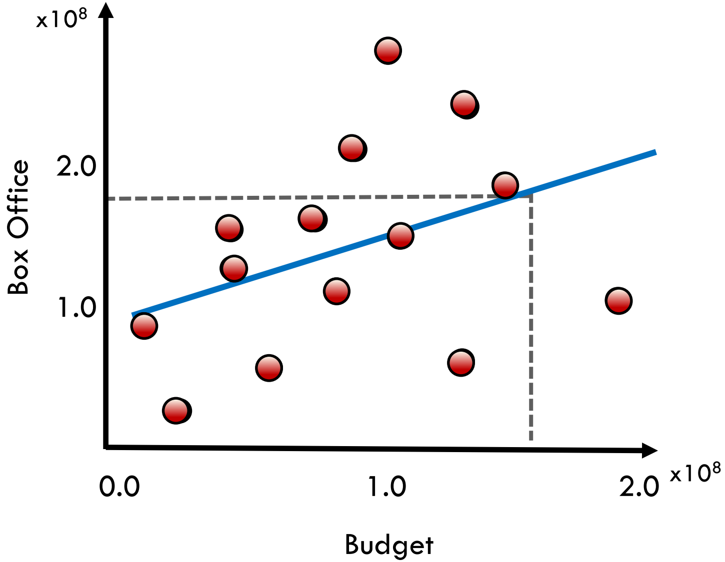
Introduction to Linear Regression



$$y_\beta(x) = \beta_0 + \beta_1 x$$

$\beta_0 =$ 80 million, $\beta_1 = 0.6$

Predicting from Linear Regression

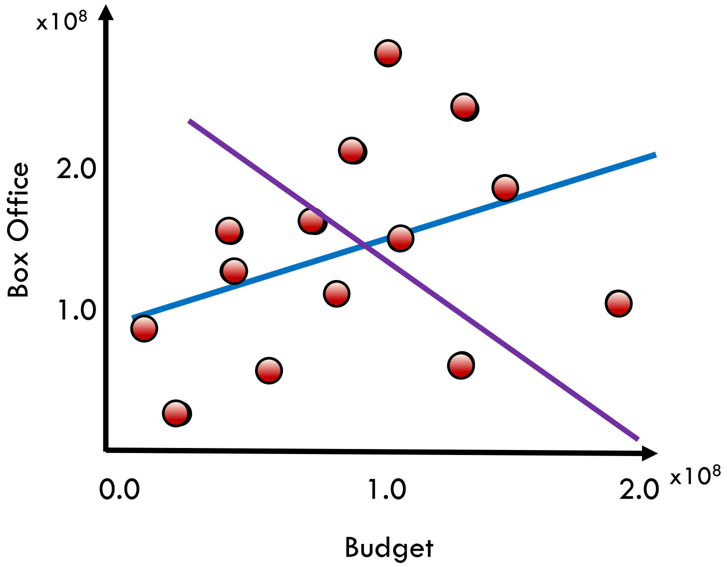


$$y_\beta(x) = \beta_0 + \beta_1 x$$

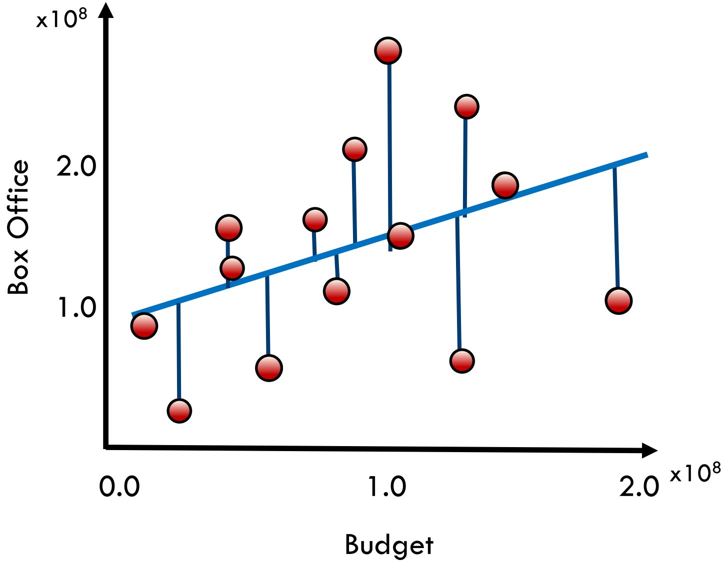
β_0= 80 million, β_1= 0.6

Predict 175 Million Gross for 160 Million Budget

Which Model Fits the Best?



Calculating the Residuals

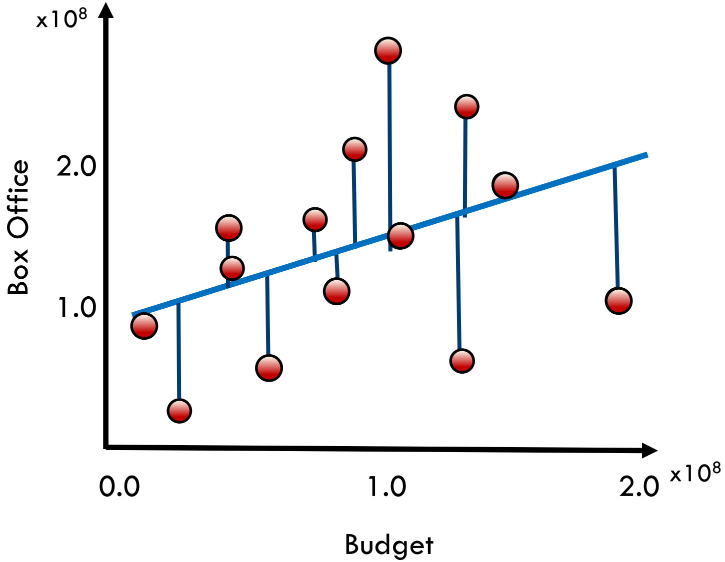


$$y_\beta\left(x_{obs}^{(i)}\right) - y_{obs}^{(i)}$$

predicted value

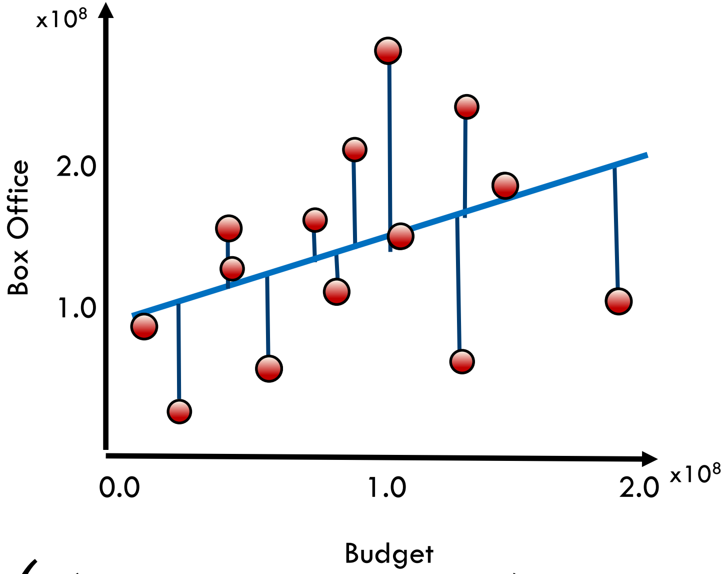
observed value

Calculating the Residuals



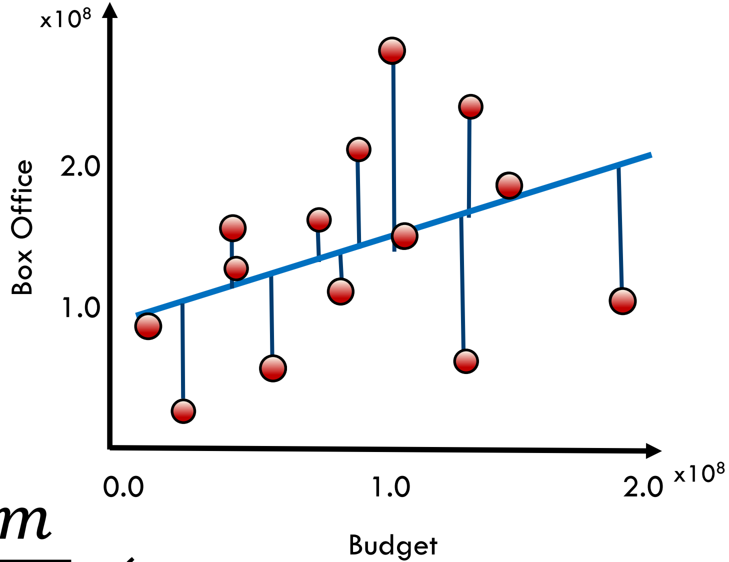
$$\left(\beta_0 + \beta_1 x_{obs}^{(i)}\right) - y_{obs}^{(i)}$$

Mean Squared Error



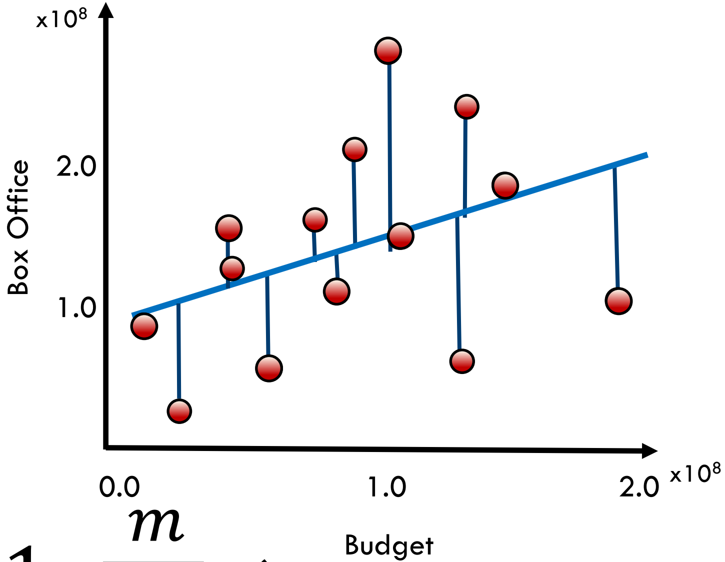
$$\frac{1}{m}\sum_{i=1}^{m}\left(\left(\beta_0 + \beta_1 x_{obs}^{(i)}\right) - y_{obs}^{(i)}\right)^2$$

Minimum Mean Squared Error



$$\min_{\beta_0,\beta_1} \frac{1}{m} \sum_{i=1}^{m} \left(\left(\beta_0 + \beta_1 x_{obs}^{(i)} \right) - y_{obs}^{(i)} \right)^2$$

Cost Function



$$J(\beta_0, \beta_1) = \frac{1}{2m} \sum_{i=1}^{m} \left(\left(\beta_0 + \beta_1 x_{obs}^{(i)} \right) - y_{obs}^{(i)} \right)^2$$

Modelling Best Practice

- Use cost function to fit model
- Develop multiple models
- Compare results and choose best one

Other Model Metrics

Sum of Squared Error (SSE): $$\sum_{i=1}^{m}\left(y_\beta(x^{(i)}) - y_{obs}^{(i)}\right)^2$$

Other Measures of Error

Sum of Squared Error (SSE): $$\sum_{i=1}^{m} \left(y_\beta(x^{(i)}) - y_{obs}^{(i)} \right)^2$$

Total Sum of Squares (TSS): $$\sum_{i=1}^{m} \left(\overline{y_{obs}} - y_{obs}^{(i)} \right)^2$$

Other Measures of Error

Sum of Squared Error (SSE): $$\sum_{i=1}^{m}\left(y_{\beta}(x^{(i)}) - y_{obs}^{(i)}\right)^2$$

Total Sum of Squares (TSS): $$\sum_{i=1}^{m}\left(\overline{y_{obs}} - y_{obs}^{(i)}\right)^2$$

Correlation Coefficient (R^2): $$1 - \frac{SSE}{TSS}$$

Comparing Linear Regression and KNN

Linear Regression	K Nearest Neighbors
• Fitting involves minimizing cost function (*slow*)	• Fitting involves storing training data (*fast*)

Comparing Linear Regression and KNN

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• Model has few parameters (*memory efficient*)	• Model has many parameters (*memory intensive*)

Comparing Linear Regression and KNN

Linear Regression

- Fitting involves minimizing cost function (*slow*)
- Model has few parameters (*memory efficient*)
- Prediction involves calculation (*fast*)

K Nearest Neighbors

- Fitting involves storing training data (*fast*)
- Model has many parameters (*memory intensive*)
- Prediction involves finding closest neighbors (*slow*)

Linear Regression: The Syntax

Import the class containing the regression method

```
from sklearn.linear_model import LinearRegression
```

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Create an instance of the class

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Create an instance of the class

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LR = LinearRegression()
```

Fit the instance on the data and then predict the expected value

```
LR = LR.fit(X_train, y_train)

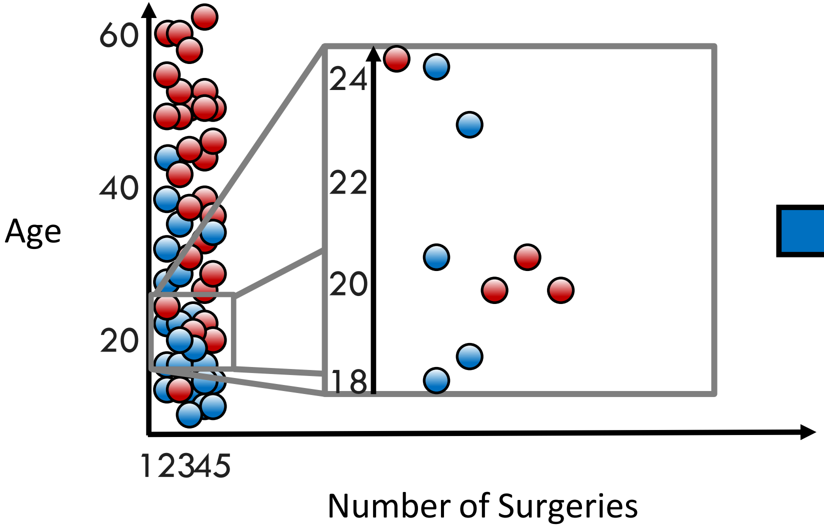
y_predict = LR.predict(X_test)
```

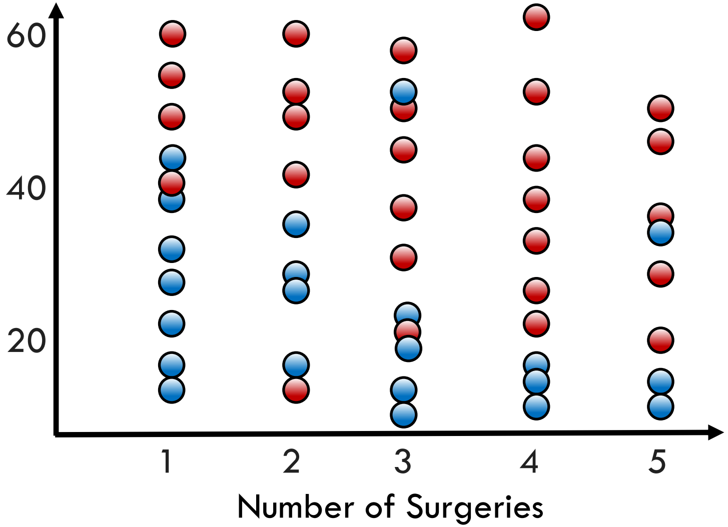
Software

Advanced

Linear Regression

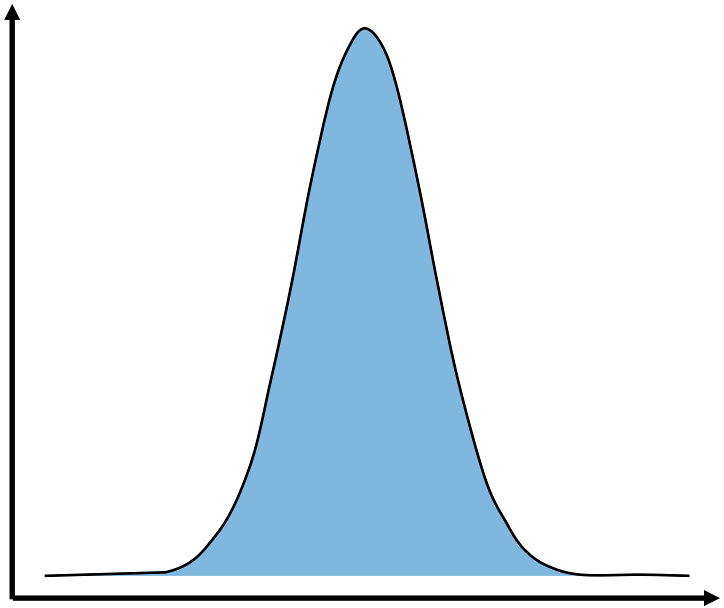
Scaling is a Type of Feature Transformation





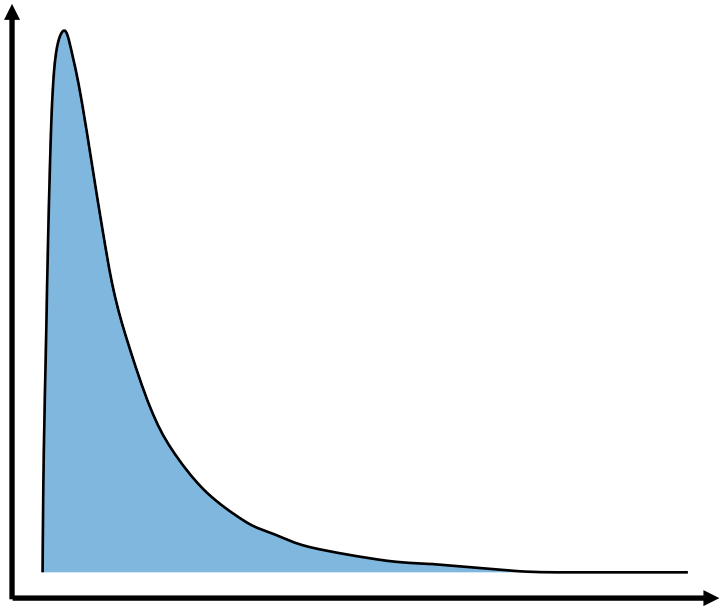
Transformation of Data Distributions

- Predictions from linear regression models assume residuals are normally distributed

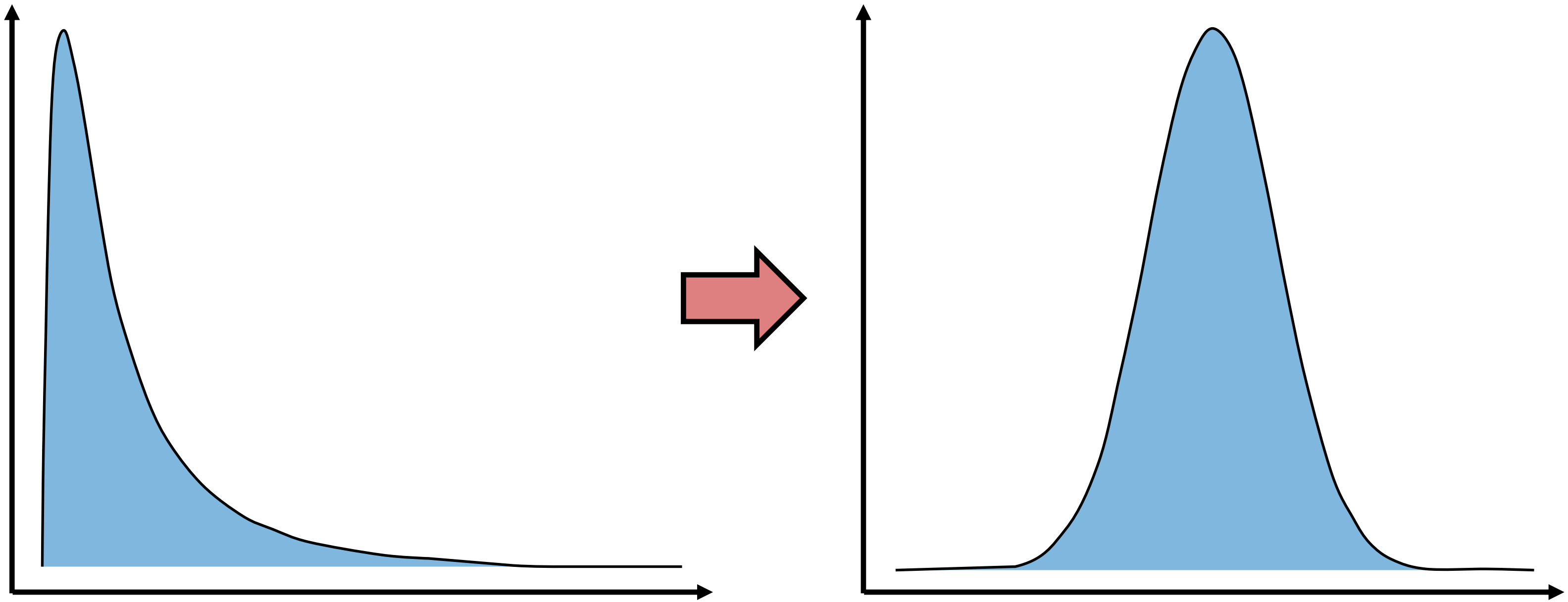


Transformation of Data Distributions

- Predictions from linear regression models assume residuals are normally distributed
- Features and predicted data are often skewed



Transformation of Data Distributions

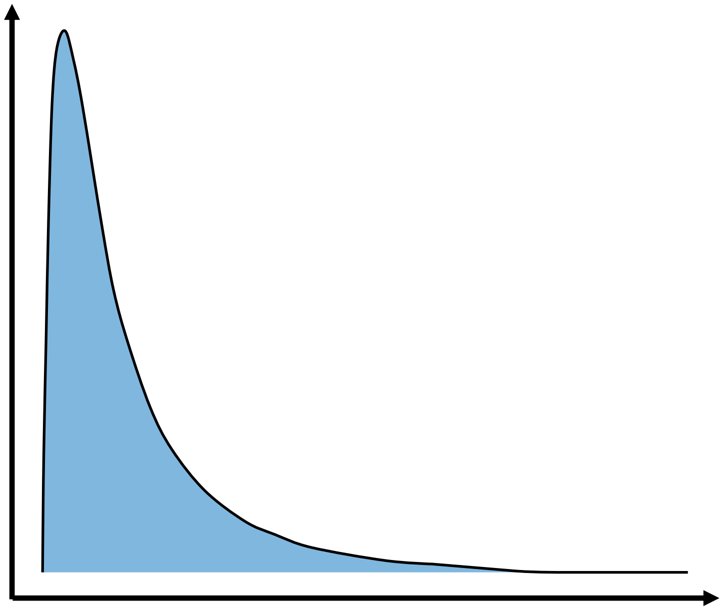


```
from numpy import log, log1p

from scipy.stats import boxcox
```

Transformation of Data Distributions

- Predictions from linear regression models assume residuals are normally distributed
- Features and predicted data are often skewed
- Data transformations can solve this issue



Feature Types

Feature Type	Transformation
• **Continuous:** numerical values	

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Feature Types

Feature Type	Transformation
• **Continuous:** numerical values	• Standard Scaling, Min-Max Scaling
• **Nominal:** categorical, unordered features (*True* or *False*)	• One-hot encoding (0, 1)

from sklearn.preprocessing import LabelEncoder, LabelBinarizer, OneHotEncoder

Feature Types

Feature Type	Transformation
• **Continuous:** numerical values	• Standard Scaling, Min-Max Scaling
• **Nominal:** categorical, unordered features (*True* or *False*)	• One-hot encoding (0, 1)
• **Ordinal:** categorical, ordered features (movie ratings)	• Ordinal encoding (0, 1, 2, 3)

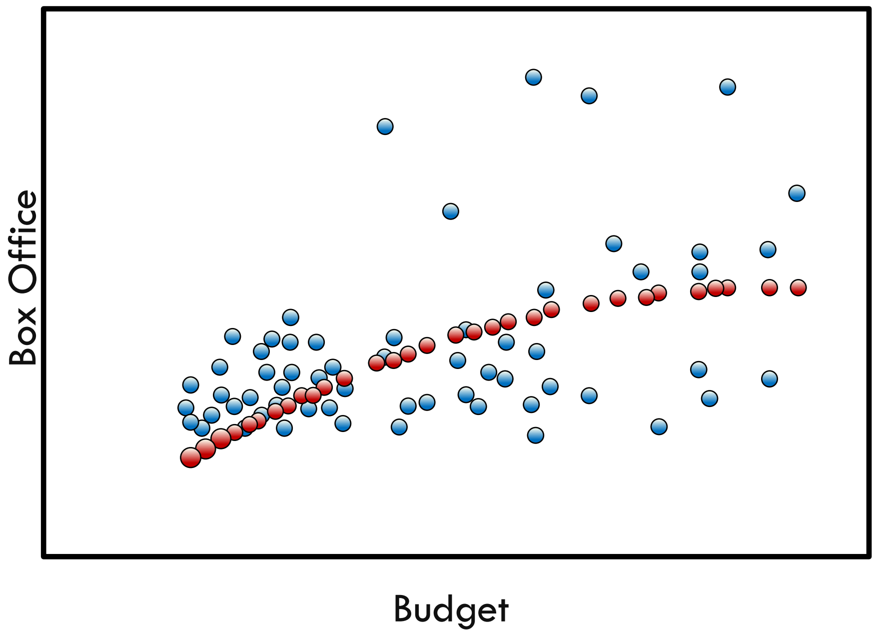
from sklearn.feature_extraction import DictVectorizer

from pandas import get_dummies

Addition of Polynomial Features

$$y_\beta(x) = \beta_0 + \beta_1 x + \beta_2 x^2$$

- Capture higher order features of data by adding polynomial features

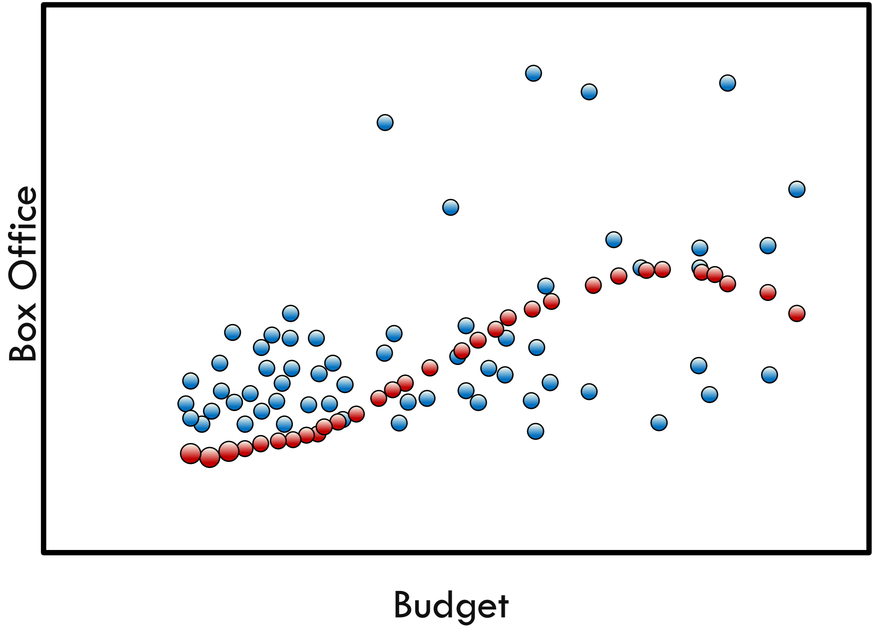


Addition of Polynomial Features

$$y_\beta(x) = \beta_0 + \beta_1 x + \beta_2 x^2 + \beta_3 x^3$$

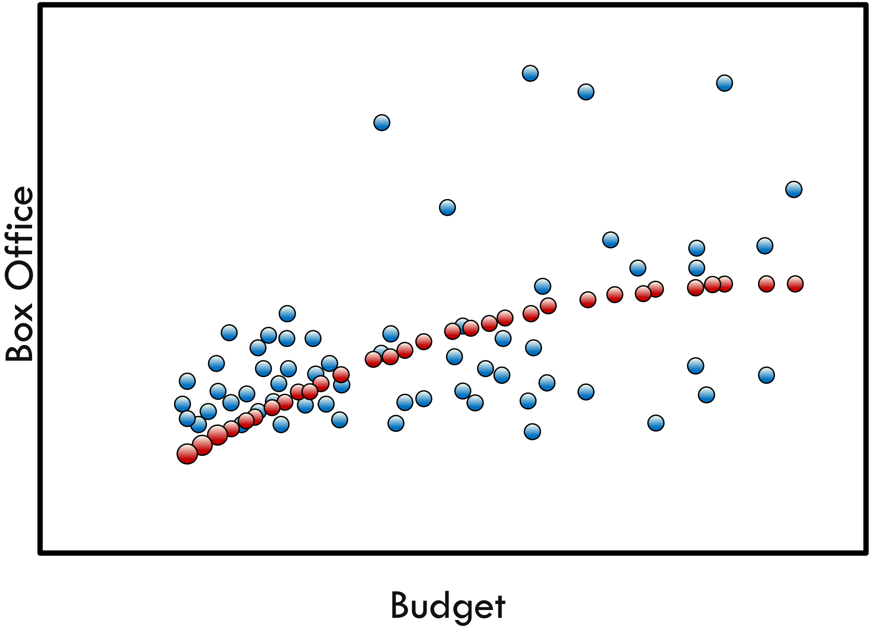
- Capture higher order features of data by adding polynomial features

- "Linear regression" means linear combinations of features



Addition of Polynomial Features

$$y_\beta(x) = \beta_0 + \beta_1 x + \beta_2 x^2$$



- Capture higher order features of data by adding polynomial features

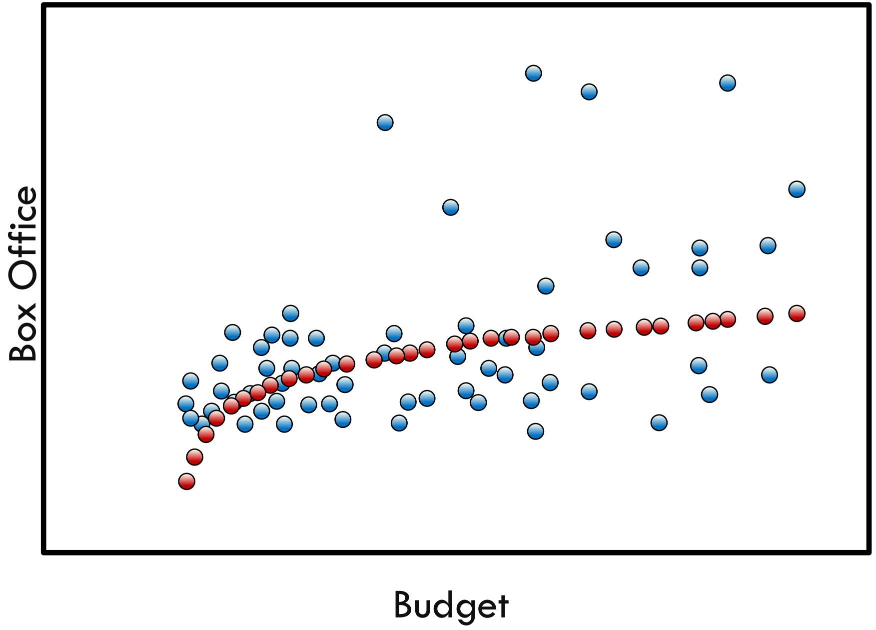
- "Linear regression" means linear combinations of features

Addition of Polynomial Features

$$y_\beta(x) = \beta_0 + \beta_1 \log(x)$$

- Capture higher order features of data by adding polynomial features

- "Linear regression" means linear combinations of features



Addition of Polynomial Features

- Can also include variable interactions

$$y_\beta(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2$$

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Addition of Polynomial Features

- Can also include variable interactions

$$y_\beta(x) = \beta_0 + \beta_1 x_1 + \beta_2 x_2 + \beta_3 x_1 x_2$$

- How is the correct functional form chosen?

Check relationship of each variable or with outcome

Polynomial Features: The Syntax

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from sklearn.preprocessing import PolynomialFeatures
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polyFeat = PolynomialFeatures(degree=2)
```

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Import the class containing the transformation method

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from sklearn.preprocessing import PolynomialFeatures
```

Create an instance of the class

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polyFeat = PolynomialFeatures(degree=2)
```

Create the polynomial features and then transform the data

```
polyFeat = polyFeat.fit(X_data)

X_poly = polyFeat.transform(X_data)
```

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