FIT1043 Introduction to Data Science

Week 6: Regression Analysis

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With materials from Wray Buntine, Mahsa Salehi

Week 5 Coverage Models Machine Learning

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Models and Machine Learning

Week 5 Coverage

Models

What is model?

What are predictive models?

How to evaluate predictive models?

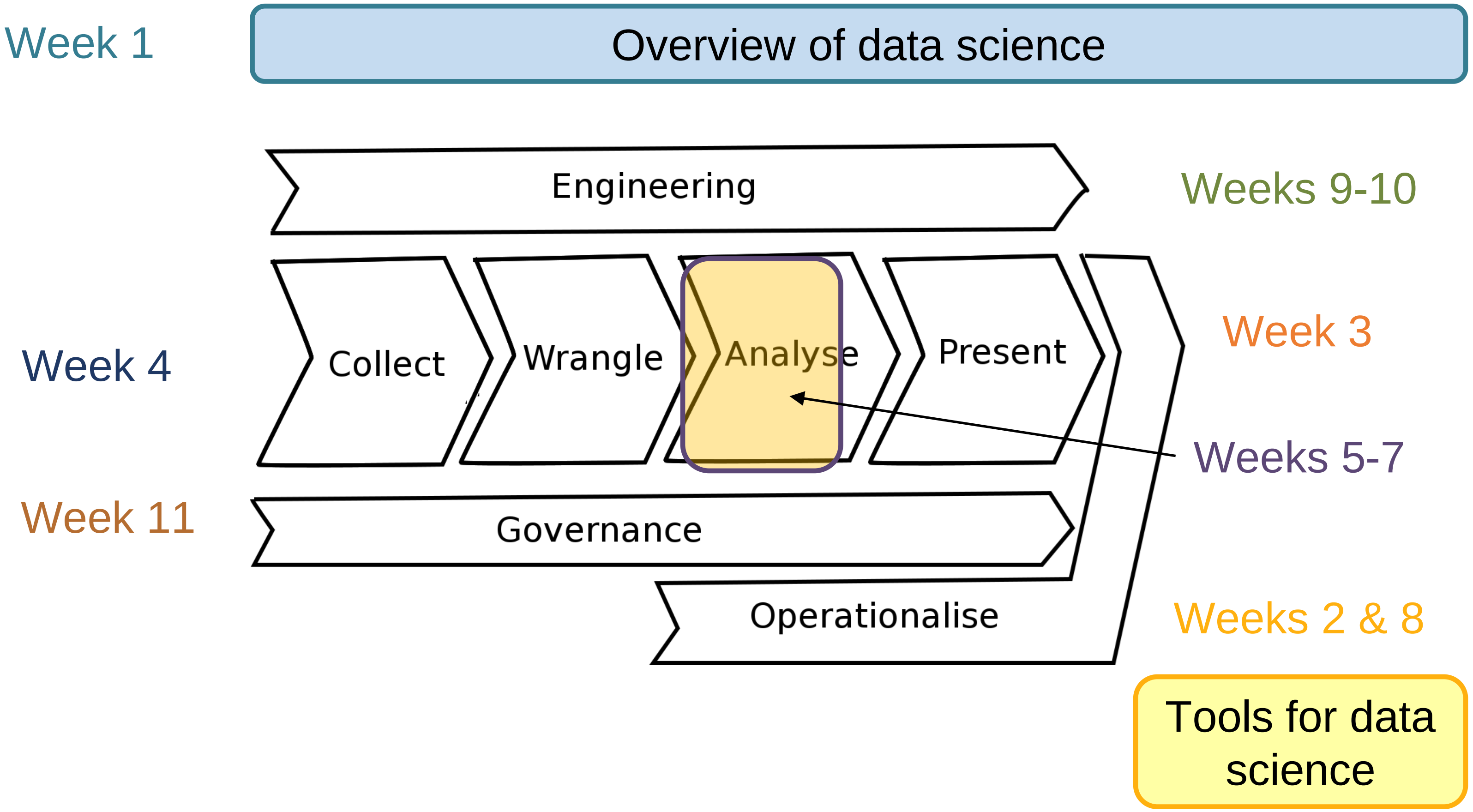
Machine Learning

Machine learning styles

What is learning theory

Linear Regression

Polynomial regression



Week 1

Overview of data science

Engineering

Weeks 9-10

Week 4

Collect

Wrangle

Analyse

Present

Week 3

Weeks 5-7

Week 11

Governance

Operationalise

Weeks 2 & 8

Tools for data science

Week	Activities	Assignments
1	Overview of data science	
2	Introduction to Python for data science	
3	Data visualisation and descriptive statistics	
4	Data sources and data wrangling	
5	Data analysis theory	Assignment 1
6	Regression analysis	
7	Classification and clustering	
8	Introduction to R for data science	Assignment 2
9	Characterising data and "big" data	
10	Big data processing	
11	Issues in data management	Assignment 3
12	Industry guest lecture (tentative)	

Introduction to Data Analysis

Week 6 Outline

Linear regression terminology

How to calculate model parameters

Underfitting vs Overfitting

Bias and Variance

- No free lunch theorem

Ensemble models

Learning Outcomes

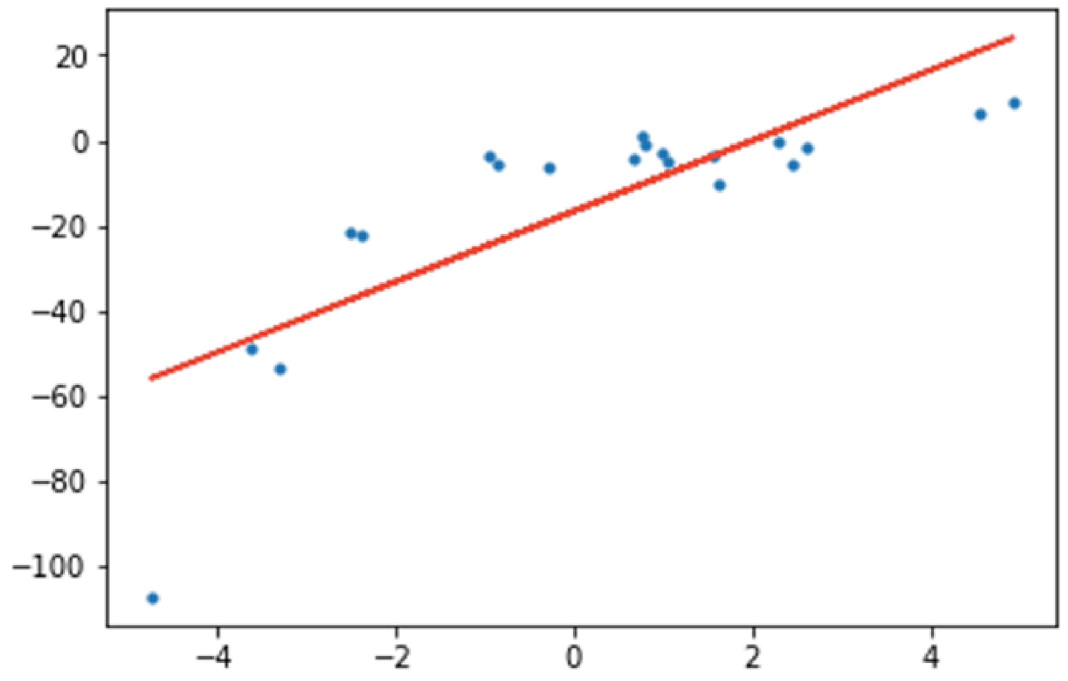
Week 6

By the end of this week you should be able to:

- Fit linear regression and polynomial regression models to a given dataset (in tutorials)
- Explain overfitting and underfitting of different models
- Comprehend bias and variance trade-off
- Comprehend the importance of “No Free Lunch Theorem”
- Explain what ensemble models are

Data Analysis Algorithms

Regression



Friedman, Jerome, Trevor Hastie, and Robert Tibshirani. The elements of statistical learning. Vol. 1, no. 10. New York: Springer series in statistics, 2001.

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Regression

What is Regression?

- The study of relationship between variables.

Examples

- Identify the relation between
  - Salary and experience, education and role
  - Exercise habits, diet and weight
  - Drinking coffee, smoking cigarettes and mortality risk

Terminology

Variables

- Independent Variables/Inputs/Predictors
  - E.g. Experience, education, role (Categorical or Continuous Data Type)

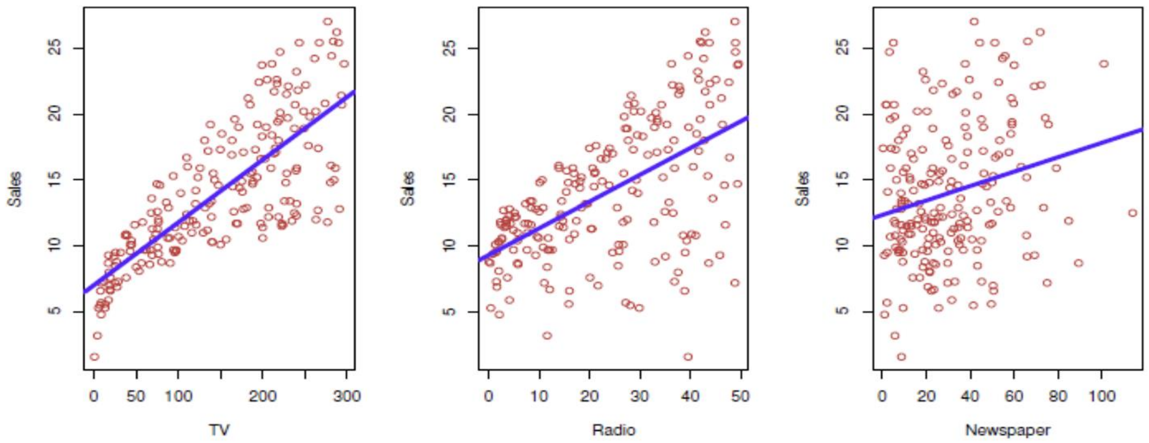
- Dependent Variables/Outputs/Responses
  - E.g. Salary of employee (Continuous Data Type)

Observations

- An observations is a data point, row, or a sample in a dataset
  - E.g., an employee's salary, experience, education, or role.

When To Use Regression

- To determine how multiple variables are related
  - E.g., determine *if* and *to what extent* the experience or education impact salaries



Example: Sales ~ TV, Radio, Newspaper

- To forecast a value
  - E.g., predict electricity consumption given the outdoor temperature, time of day, and number of residents in that household

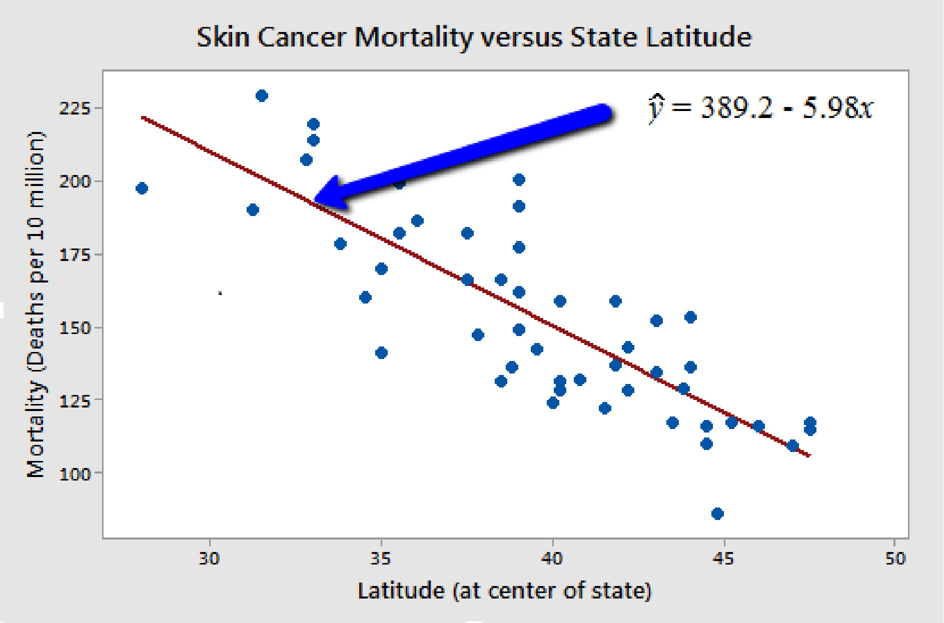
Simple Linear Regression

Two-Dimensional Space

Regression fits a very simple equation to the data:

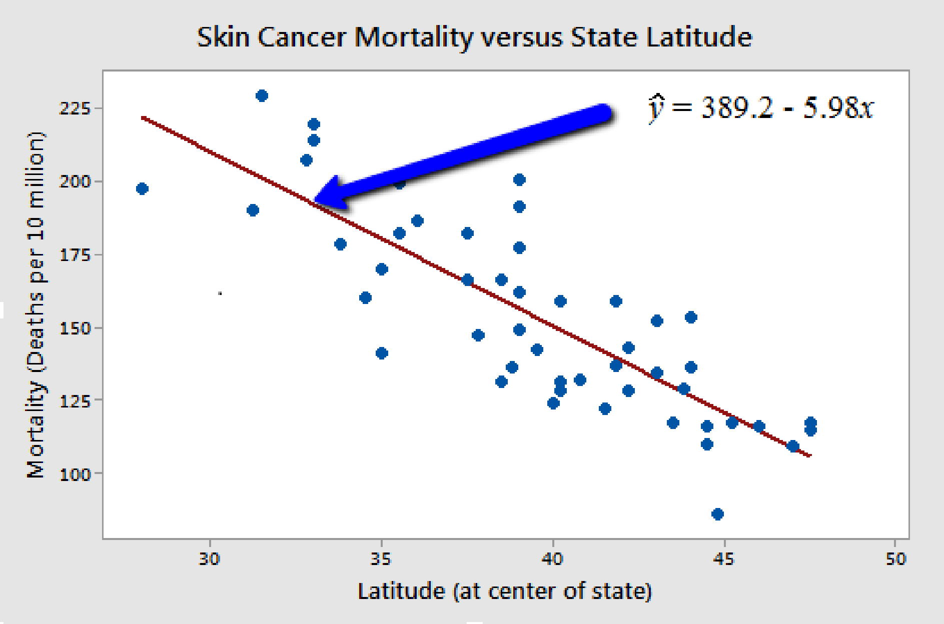
$$\hat{y}(x; \vec{a}) = a_0 + a_1 x$$

Here $\hat{y}(x; \vec{a})$ is prediction for y at the point x using the model parameters $\vec{a}$ = (a_0, a_1), i.e. the intercept and slope terms.



Simple Linear Regression

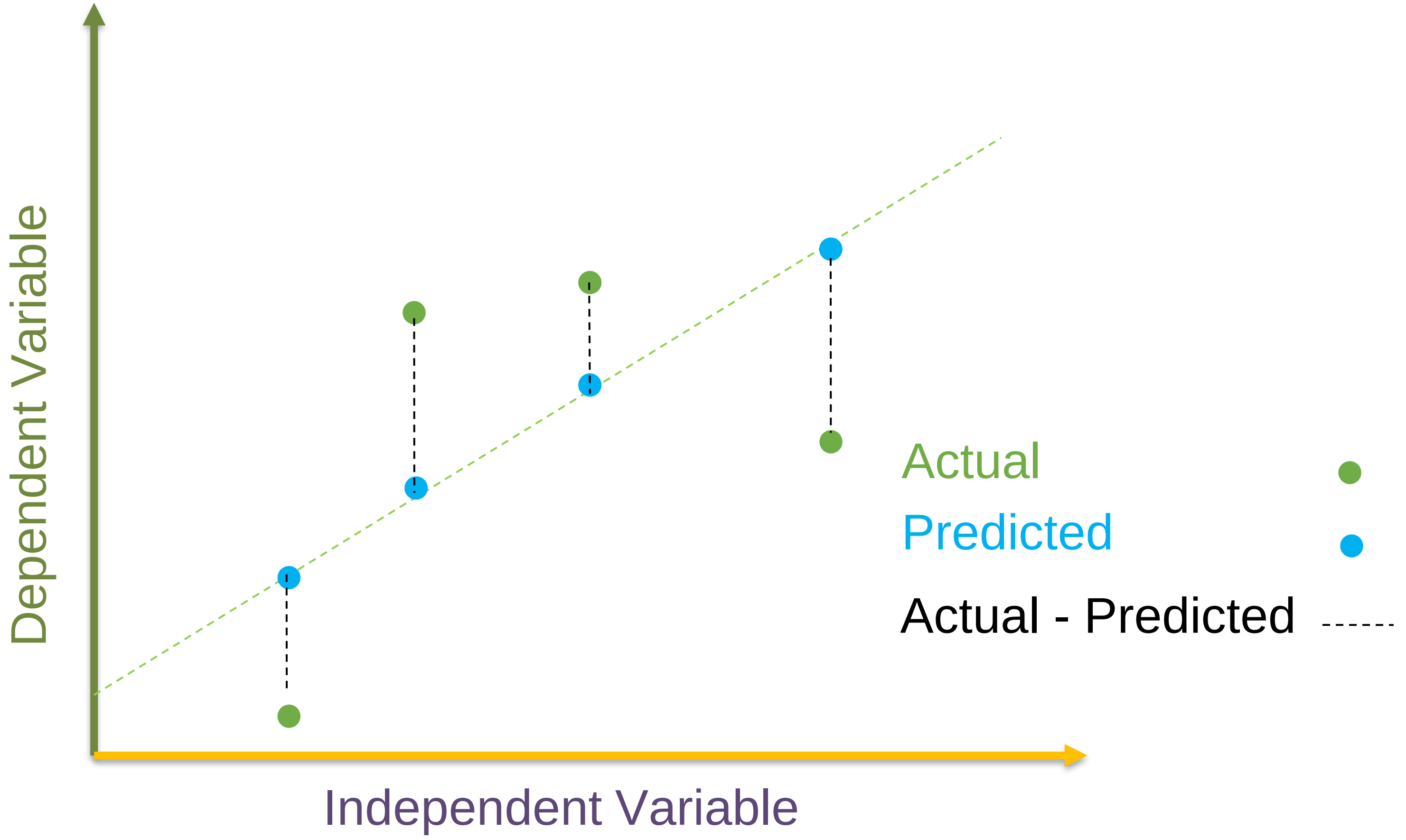
Two-Dimensional Space



Linear regression is a **linear model**,

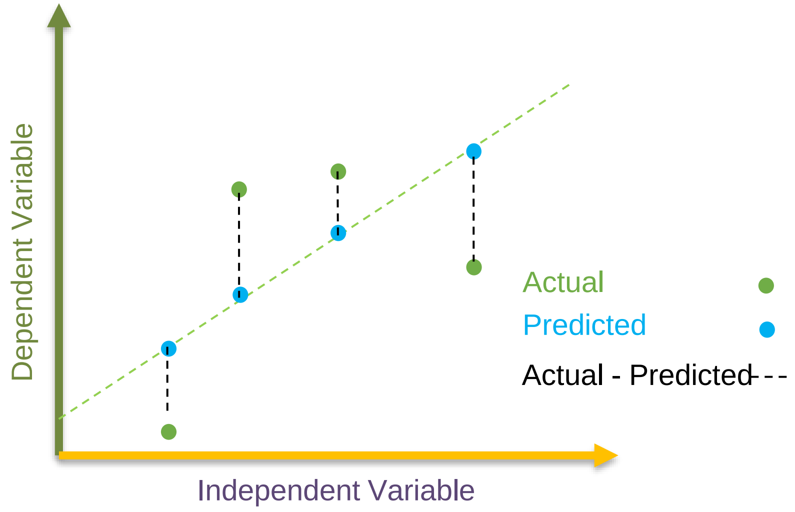
- e.g. a model that assumes a linear relationship between the input variables (x) and the single output variable (y).
- When there is a single input variable (x), the method is referred to as simple linear regression.

Best Fitting Line



The aim is for the predicted response, be as close as possible to the actual response.

Calculating the Parameters



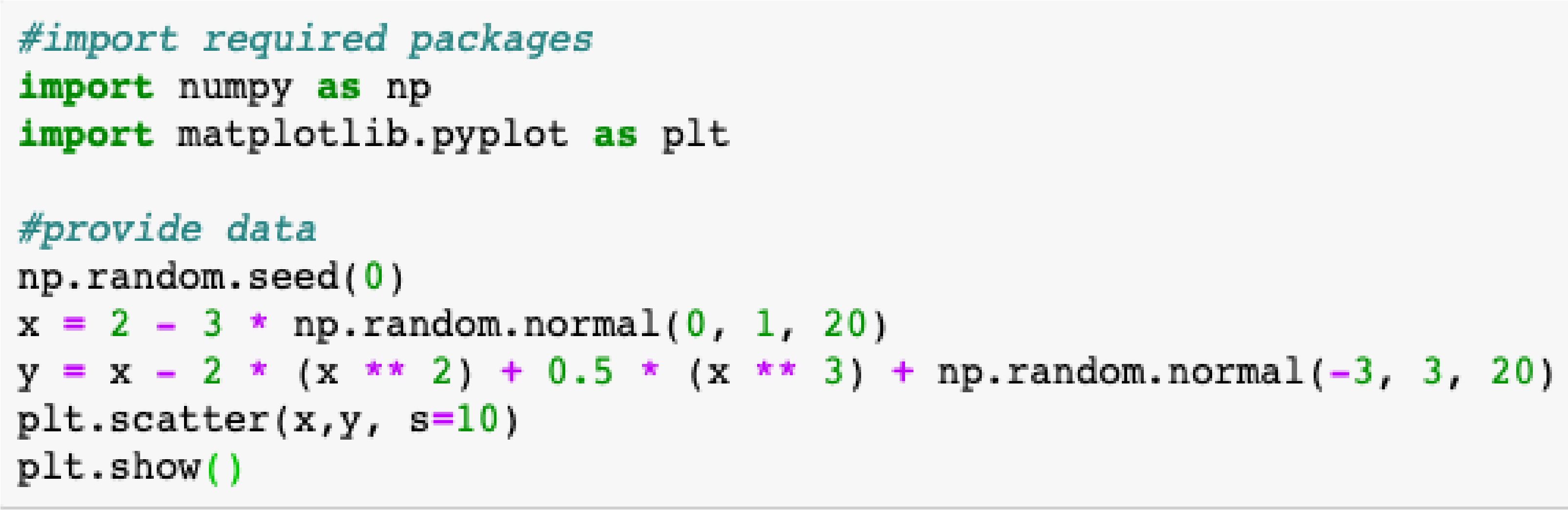
$$\hat{y}(x;\vec{a}) = a_0 + a_1 x$$

Given some data pairs (x_1, y_1), ...,$(x_N\ , y_N)$, we fit a model by finding the vector $\vec{a}$ that minimises the loss function:

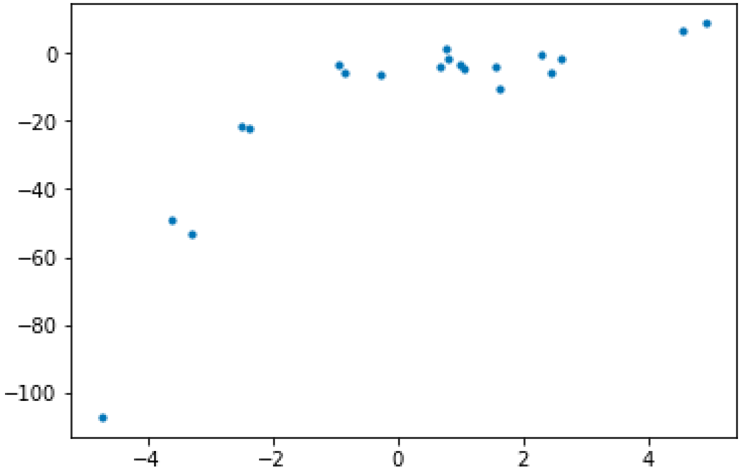
$$\text{mean square error} = MSE_{train} = \frac{1}{N}\sum_{i=1}^{N}\left(\hat{y}(x_i;\vec{a}) - y_i\right)^2$$

The mean squared error (MSE) **tells you how close a regression line is to a set of points**.

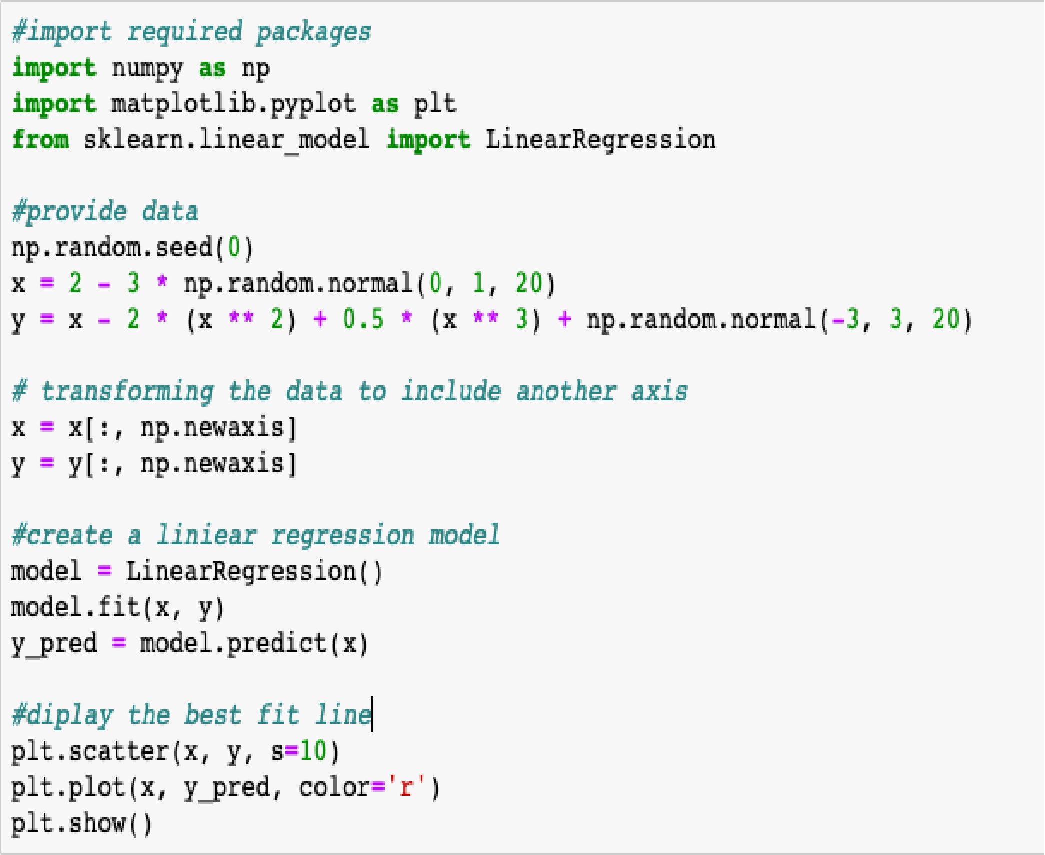
Python Example



```
#import required packages
import numpy as np
import matplotlib.pyplot as plt

#provide data
np.random.seed(0)
x = 2 - 3 * np.random.normal(0, 1, 20)
y = x - 2 * (x ** 2) + 0.5 * (x ** 3) + np.random.normal(-3, 3, 20)
plt.scatter(x,y, s=10)
plt.show()
```

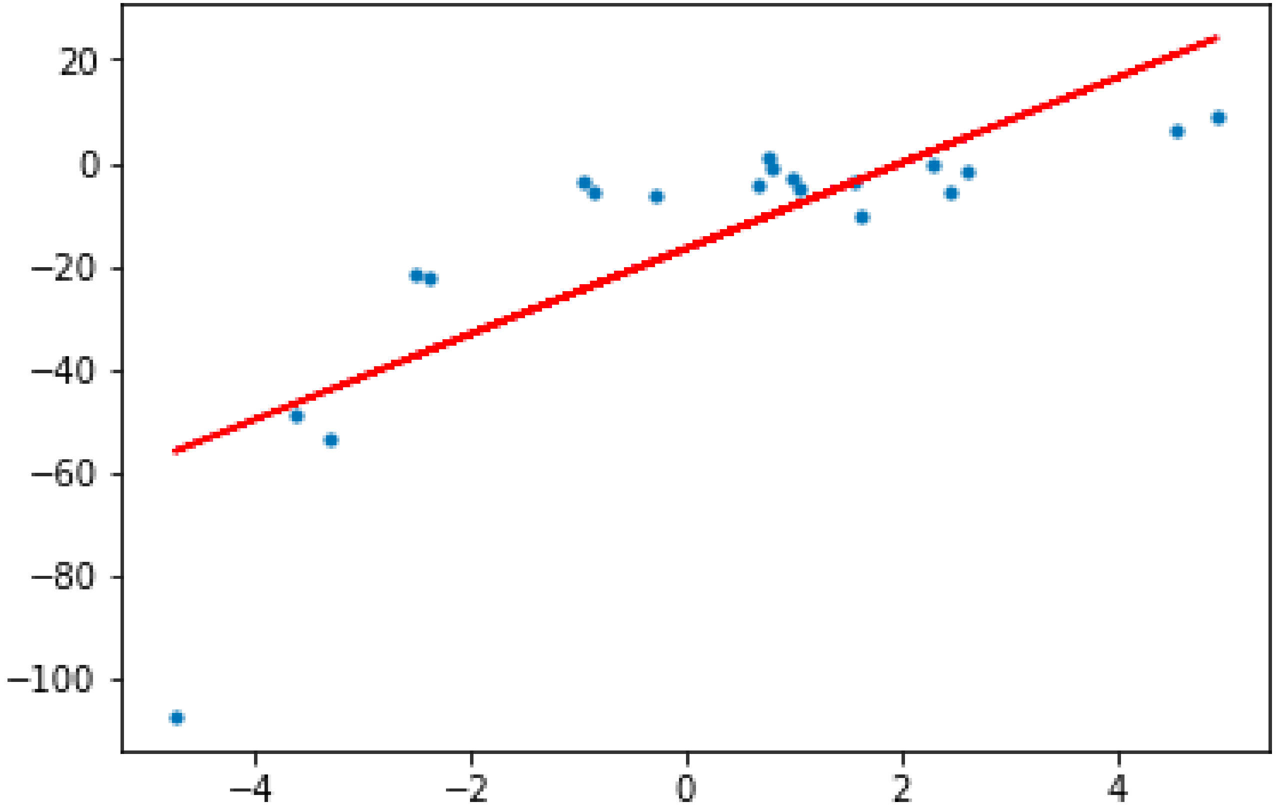


Python Example



```
#import required packages
import numpy as np
import matplotlib.pyplot as plt
from sklearn.linear_model import LinearRegression

#provide data
np.random.seed(0)
x = 2 - 3 * np.random.normal(0, 1, 20)
y = x - 2 * (x ** 2) + 0.5 * (x ** 3) + np.random.normal(-3, 3, 20)

# transforming the data to include another axis
x = x[:, np.newaxis]
y = y[:, np.newaxis]

#create a liniear regression model
model = LinearRegression()
model.fit(x, y)
y_pred = model.predict(x)

#diplay the best fit line
plt.scatter(x, y, s=10)
plt.plot(x, y_pred, color='r')
plt.show()
```

Linear regression is unable to capture the patterns in the data. This is an example of under-fitting.



To overcome under-fitting, we need to increase the complexity of the model

Python Polynomial Regression

To overcome under-fitting, we need to increase the complexity of the model

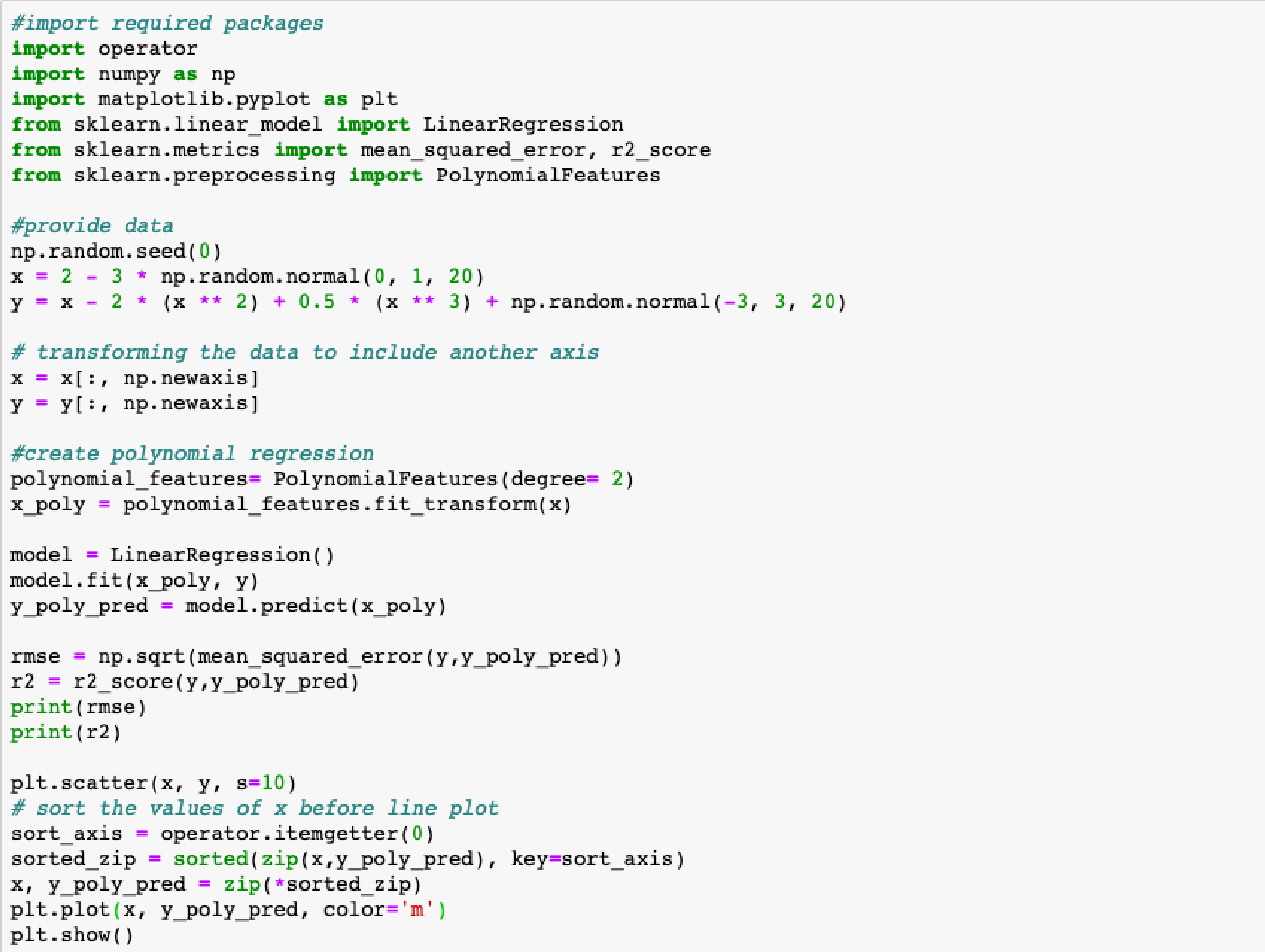
Assume the polynomial relationship between the inputs and output.

- E.g., 10th order (aka degree) polynomial

$$\hat{y}(x;\vec{a}) = a_0 + a_1 x$$

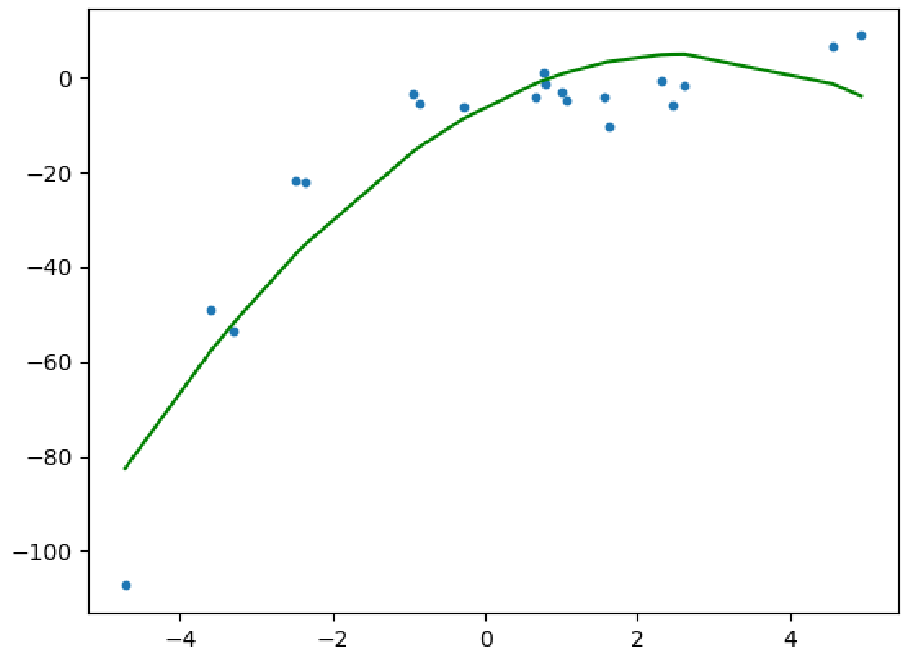
Python Polynomial Regression

2nd Degree Polynomial (Polynomial of order 2)



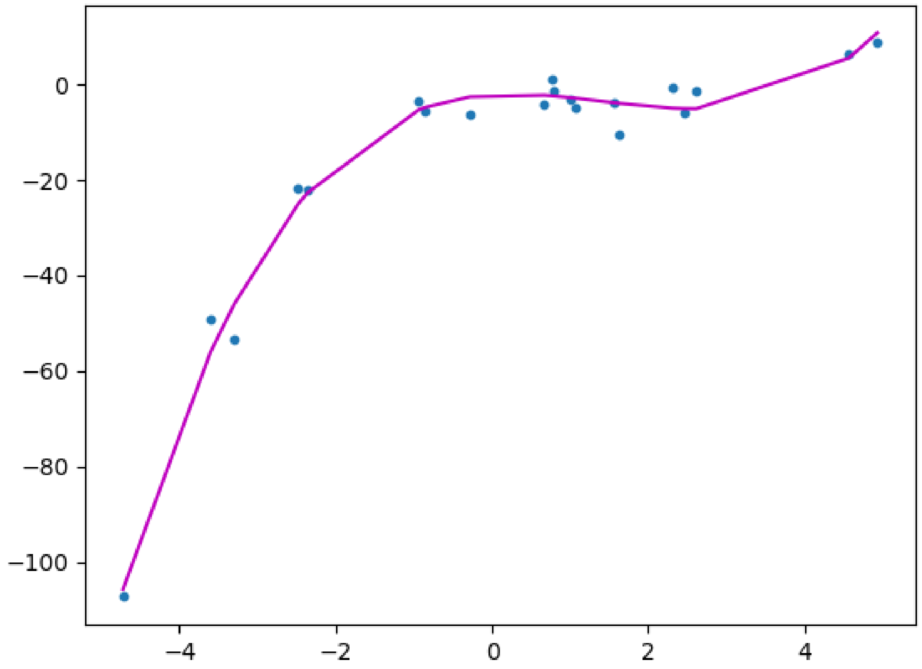
```
#import required packages
import operator
import numpy as np
import matplotlib.pyplot as plt
from sklearn.linear_model import LinearRegression
from sklearn.metrics import mean_squared_error, r2_score
from sklearn.preprocessing import PolynomialFeatures

#provide data
np.random.seed(0)
x = 2 - 3 * np.random.normal(0, 1, 20)
y = x - 2 * (x ** 2) + 0.5 * (x ** 3) + np.random.normal(-3, 3, 20)

# transforming the data to include another axis
x = x[:, np.newaxis]
y = y[:, np.newaxis]

#create polynomial regression
polynomial_features= PolynomialFeatures(degree= 2)
x_poly = polynomial_features.fit_transform(x)

model = LinearRegression()
model.fit(x_poly, y)
y_poly_pred = model.predict(x_poly)

rmse = np.sqrt(mean_squared_error(y,y_poly_pred))
r2 = r2_score(y,y_poly_pred)
print(rmse)
print(r2)

plt.scatter(x, y, s=10)
# sort the values of x before line plot
sort_axis = operator.itemgetter(0)
sorted_zip = sorted(zip(x,y_poly_pred), key=sort_axis)
x, y_poly_pred = zip(*sorted_zip)
plt.plot(x, y_poly_pred, color='m')
plt.show()
```

$$\hat{y}(x;\vec{a}) = a_0 + a_1 x + a_2 x^2$$



Python Polynomial Regression

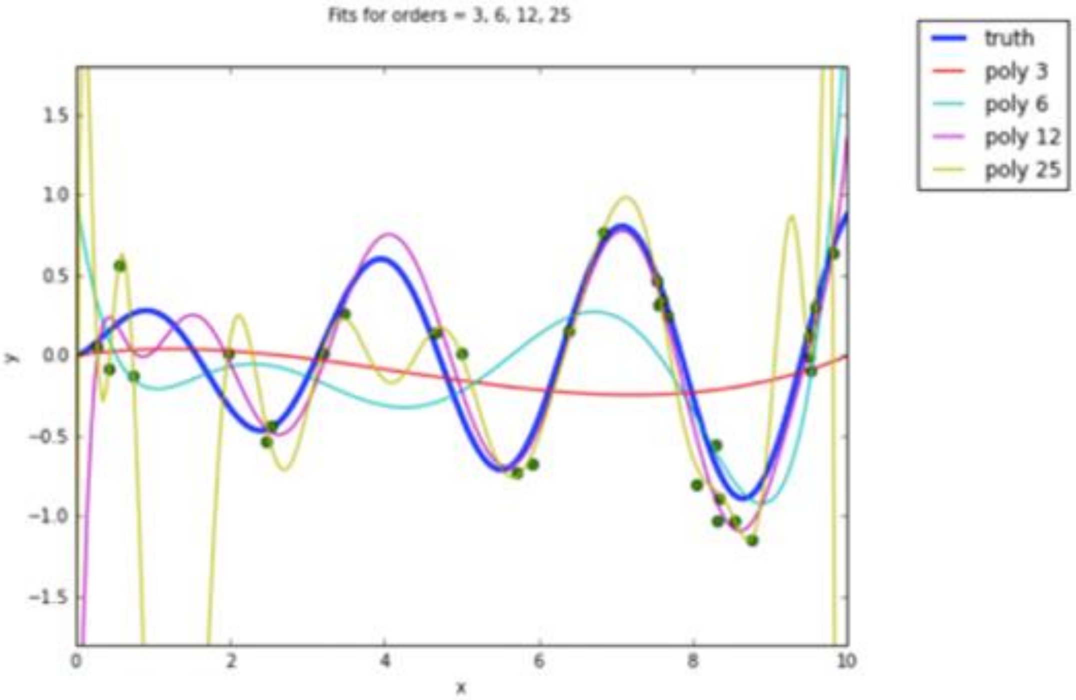
3rd Degree Polynomial (Polynomial of order 3)



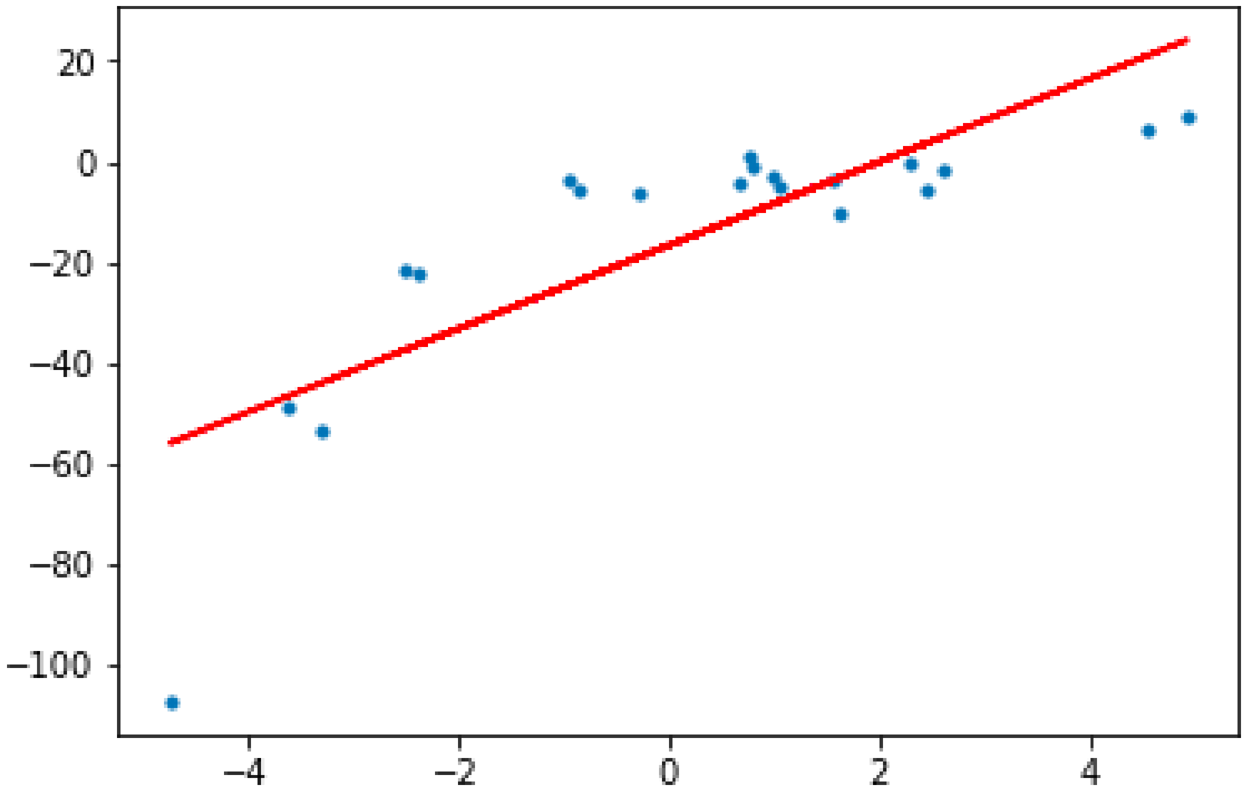
$$\hat{y}(x;\vec{a}\,) = a_0 + a_1 x \quad + a_2 x^2 + a_3 x^3$$

Underfitting and Overfitting

Model Fitting



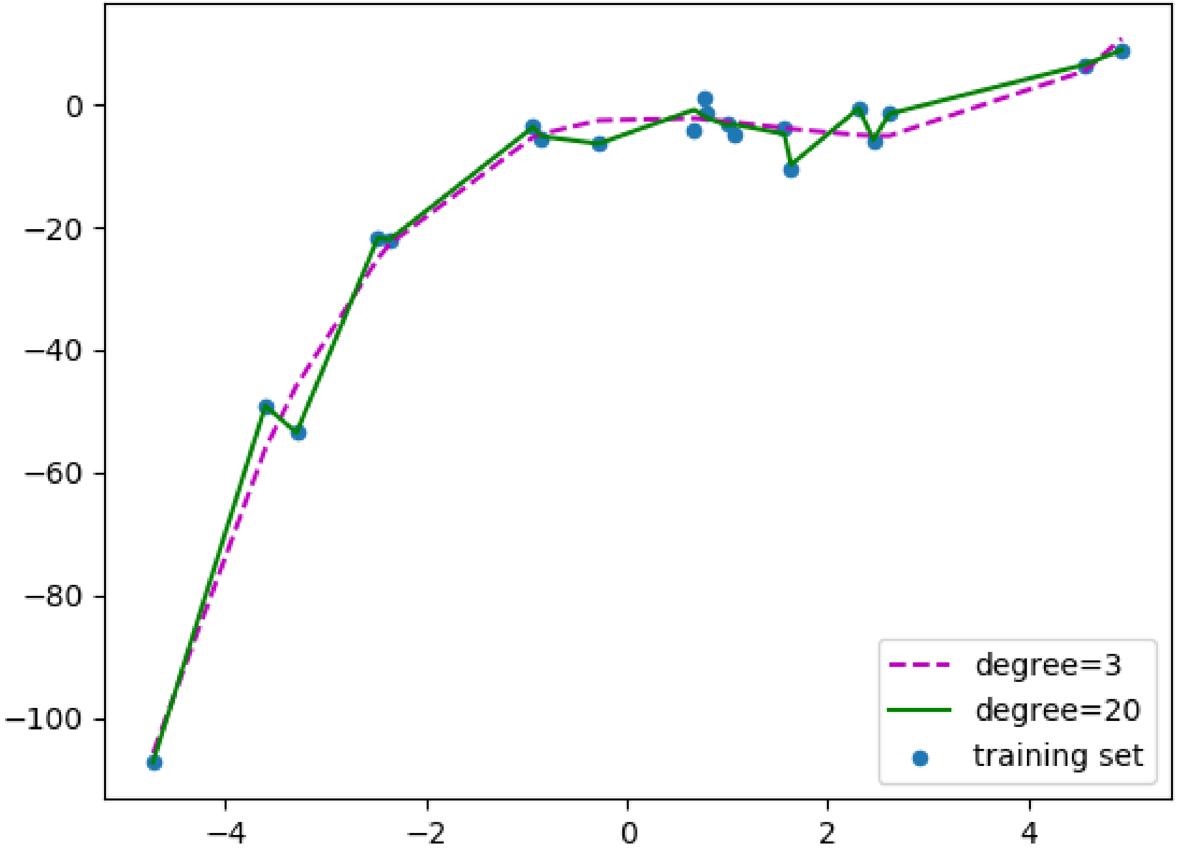
Underfitting and Overfitting



Under-Fitting

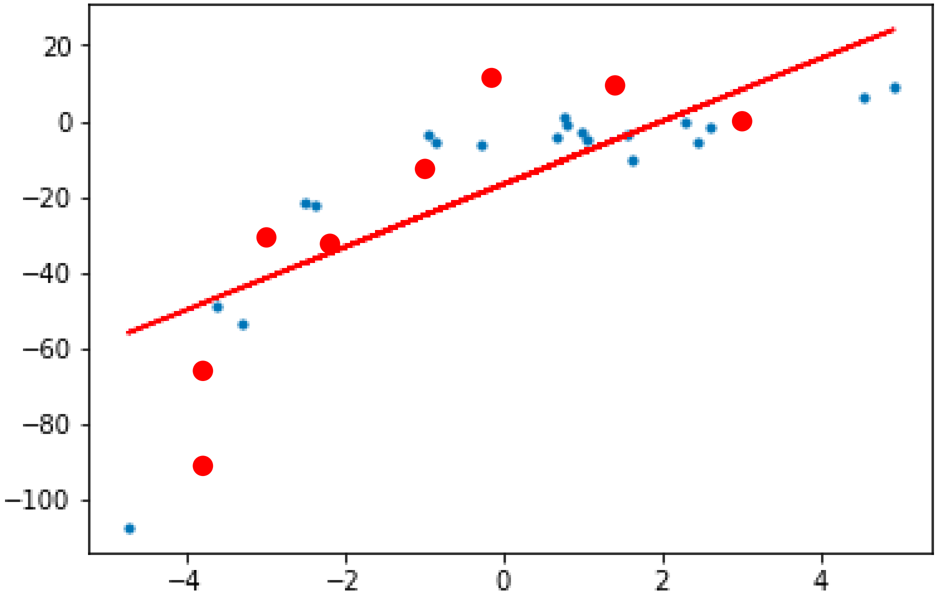
Underfitting occurs when a statistical model or machine learning algorithm cannot adequately capture the underlying structure of the data. It occurs when the model or algorithm does not fit the data enough.

Underfitting and Overfitting



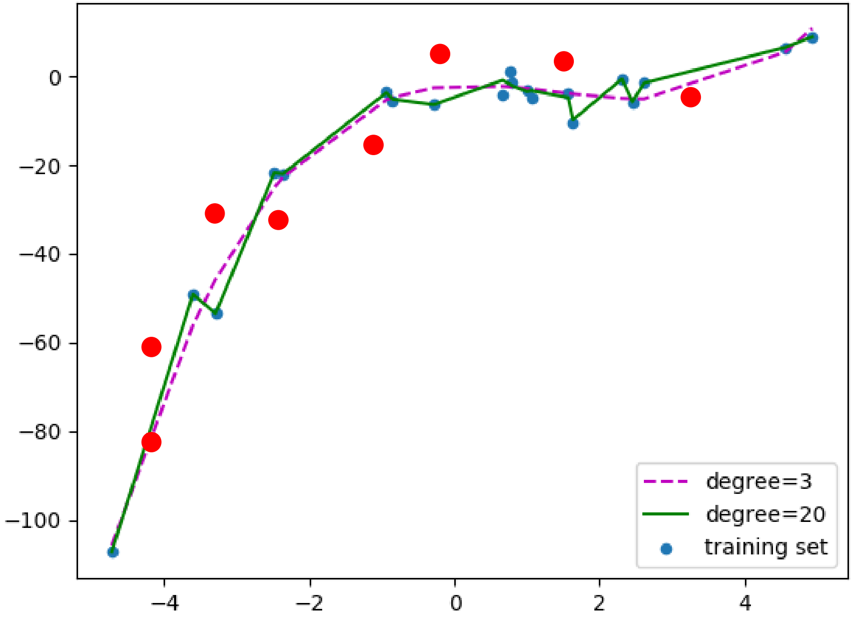
Over-Fitting

Underfitting and Overfitting

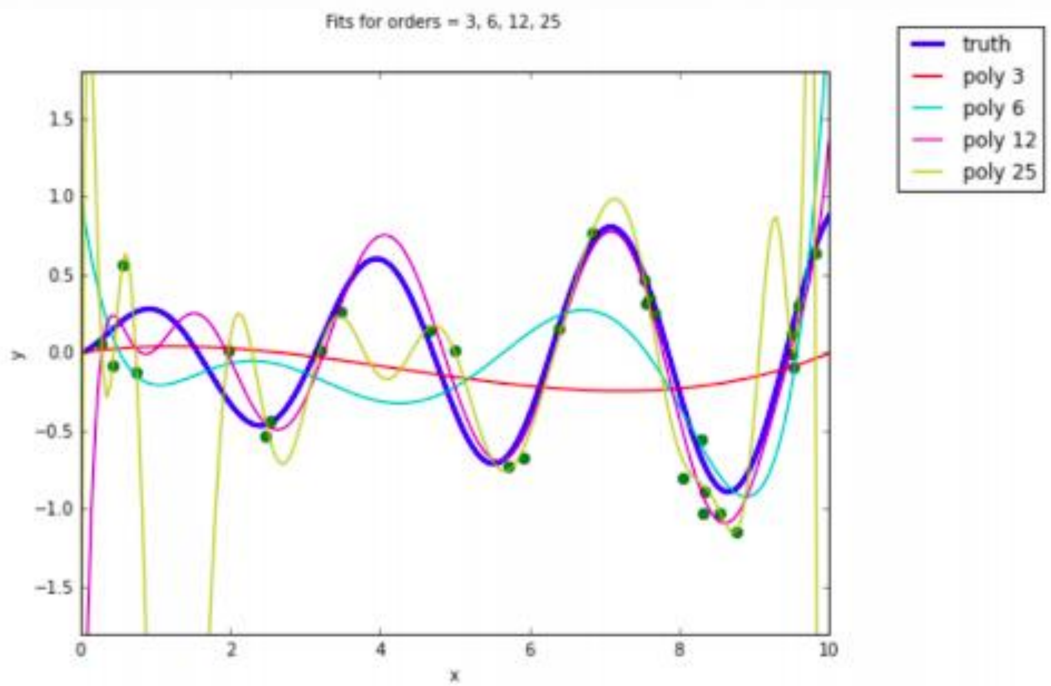


Under-Fitting

Over-Fitting



Overfitting

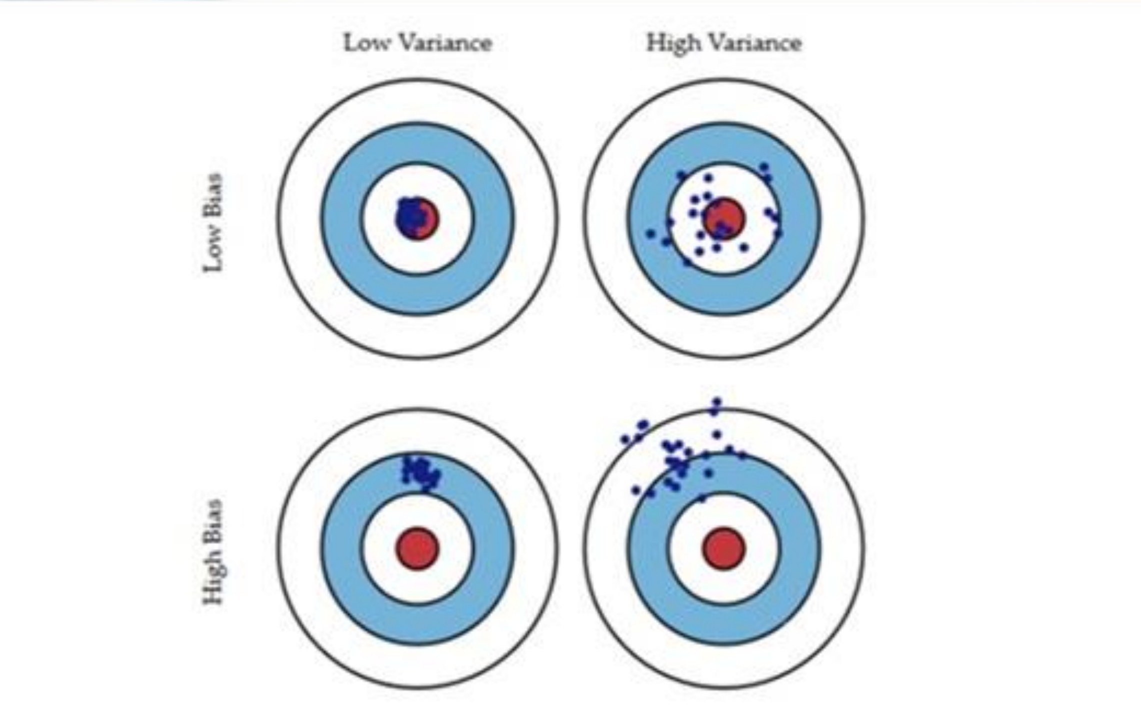


- The more parameters a model has, the more complicated a curve it can fit.
  - If we don’t have very much data and we try to fit a complicated model to it, the model will make wild predictions.
  - This phenomenon is referred to as overfitting

Overfitting

- Small polynomial; cannot fit the data well; said to have high bias
- Large polynomial; can fit the data well; fits the data too well; said to have small bias
- If there is known error in the data, then a close fit is wasted:
- 25th degree polynomial does all sorts of wild contortions!
- Poor fit due to **high bias** called underfitting
- Poor fit due to **low bias** called overfitting

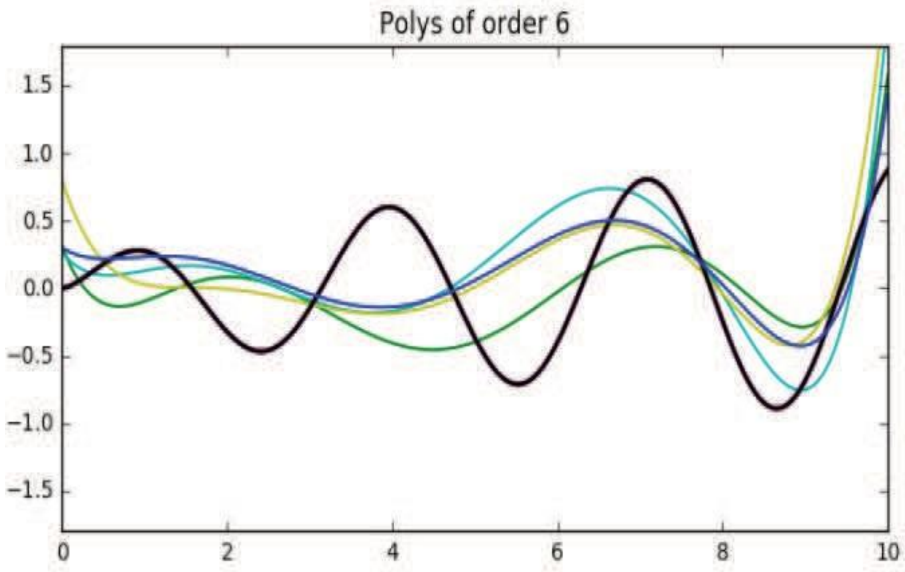
Bias and Variance



Training and Test Datasets

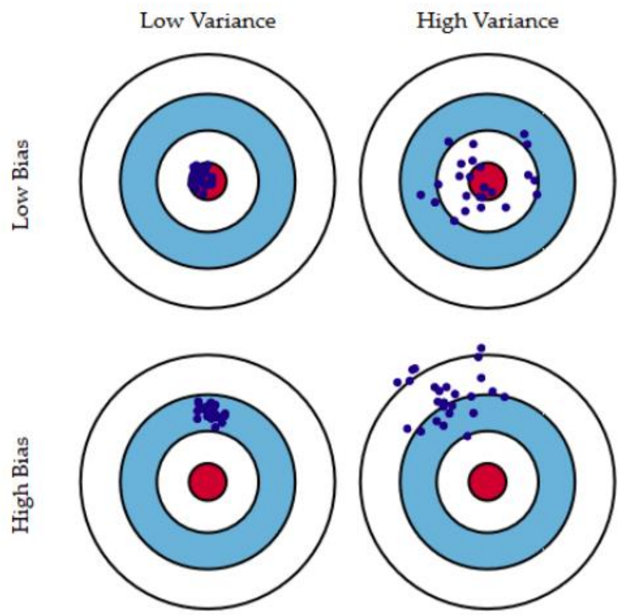
- Split up the data we have into two non-overlapping parts, a training set and a test set
- Do your learning, run your algorithm, build your model using the training set
- Run evaluation using the test set
- Don’t run evaluation on the training set
- How big to make the test set?

Bias and Variance



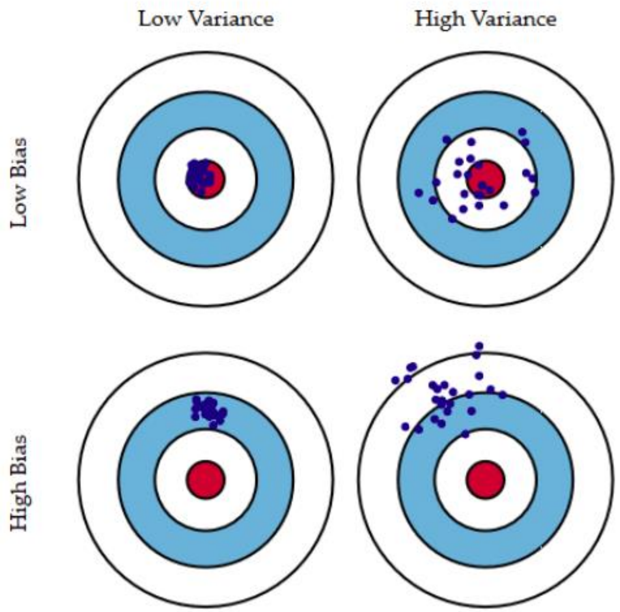
- Using different data points, the plot is for 6th degree polynomial models.
  - How do we measure how much does it differ from the desired model?
  - For each data point, does the prediction differ a lot each time?

Bias and Variance



- **Bias**: measures how much the prediction differs from the desired regression function.
- **Variance**: measures how much the predictions for individual data sets vary around their average.

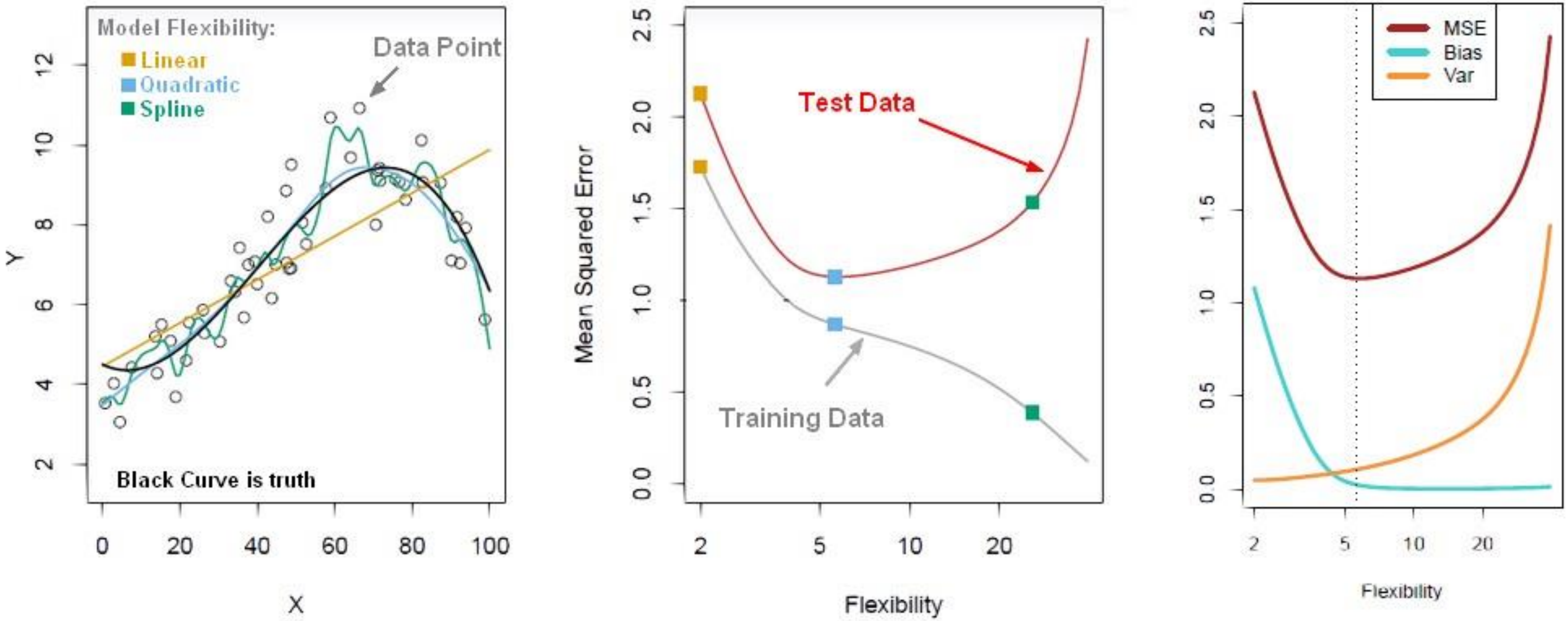
Bias and Variance



- A high bias means the prediction will be inaccurate.(underfitting)
- A high variance means that each time you predict, the results will vary widely. (overfitting)

Bias vs Variance Trade-off

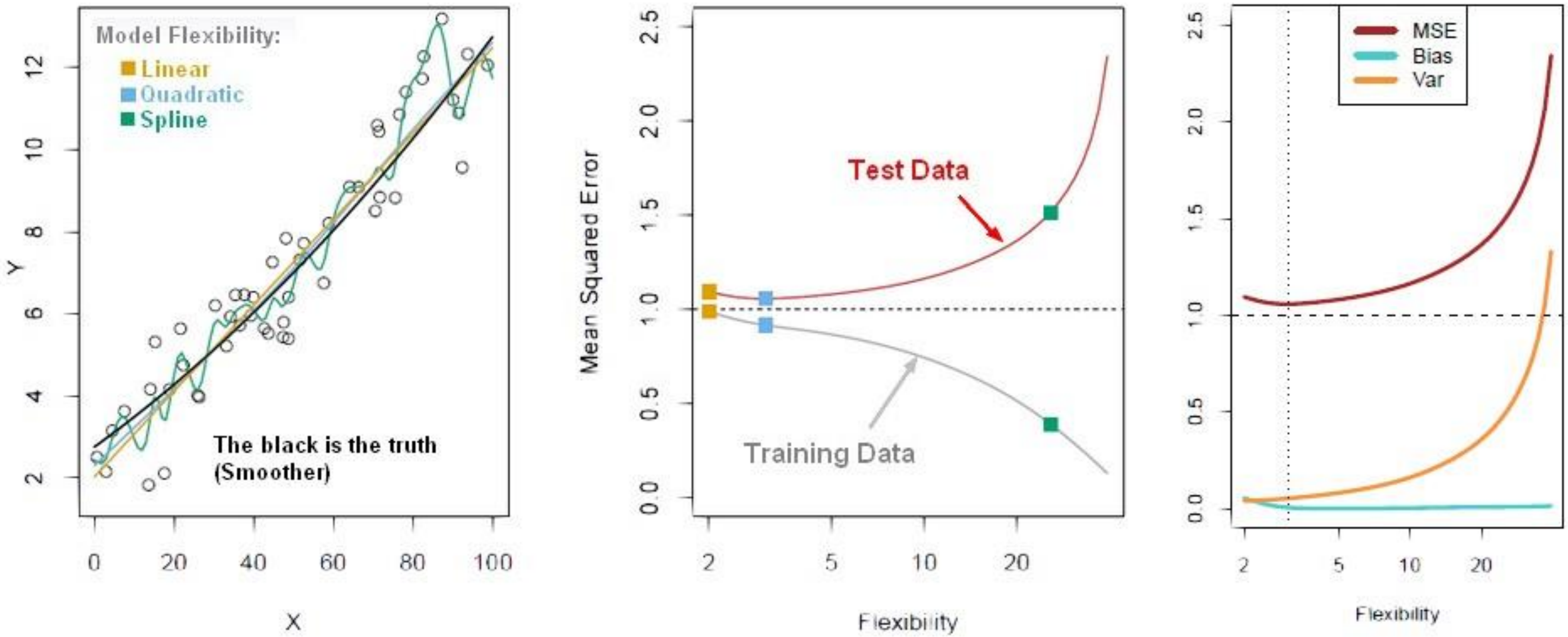
Scenario 1



- **Black line** is the truth (which is a curve) but the dots (the data points) can be quite way off from the truth values.
- **Yellow line** (the straight line) is a linear model
- **Blue** is a slightly more complex model, looks like a 5th Order, and
- **Green line** is a much more complex model

Bias vs Variance Trade-off

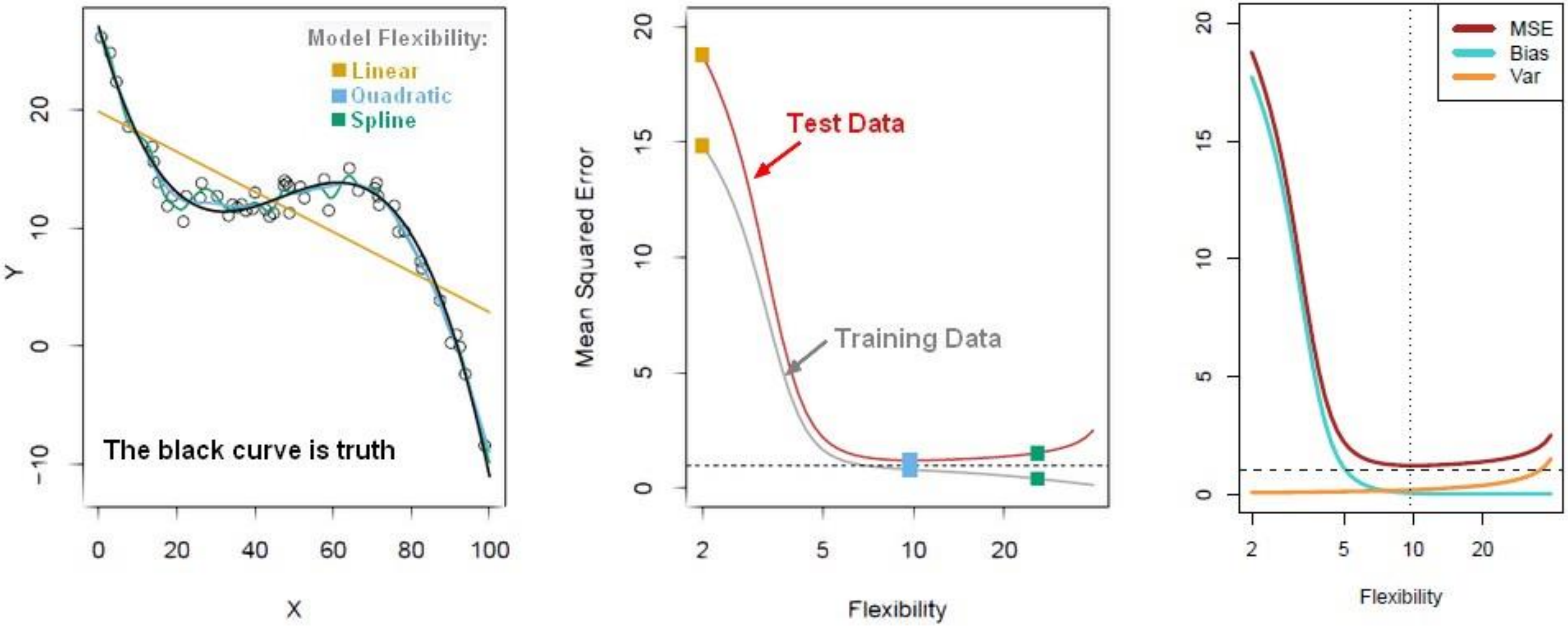
Scenario 2



- Another example where the truth function is actually very smooth, almost straight line and the data points are quite random.
- The lower complexity seems to fit very well, linear regression is just slightly worse off than the 3rd order polynomial.

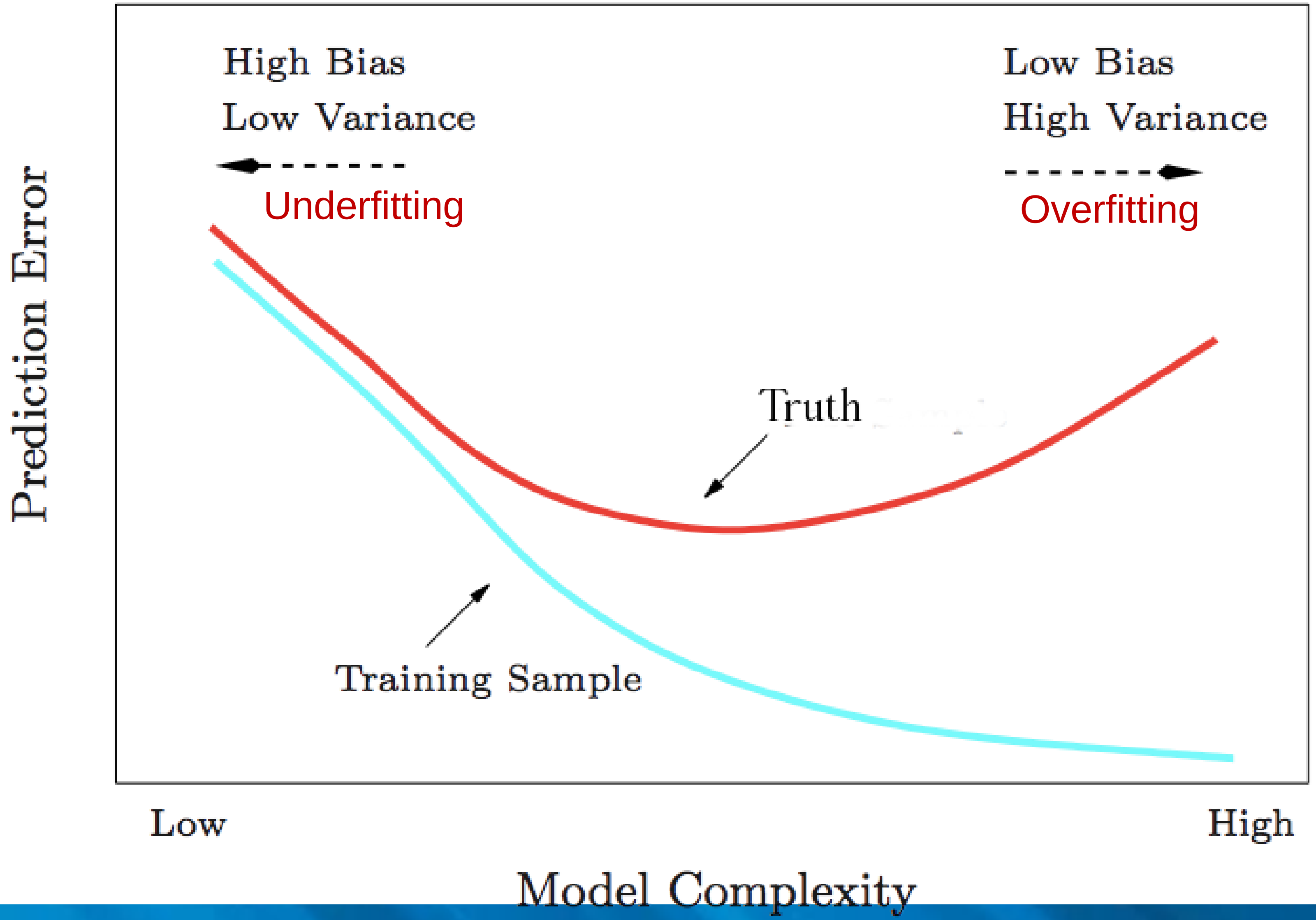
Bias vs Variance Trade-off

Scenario 3



- For this, the linear model does a poor job because it is not a straight or near straight line, hence the MSE is high.
- The complex models do better, in this case the 10th and the 23rd order polynomials.

Bias vs Variance Trade-off



No Free Lunch Theorem

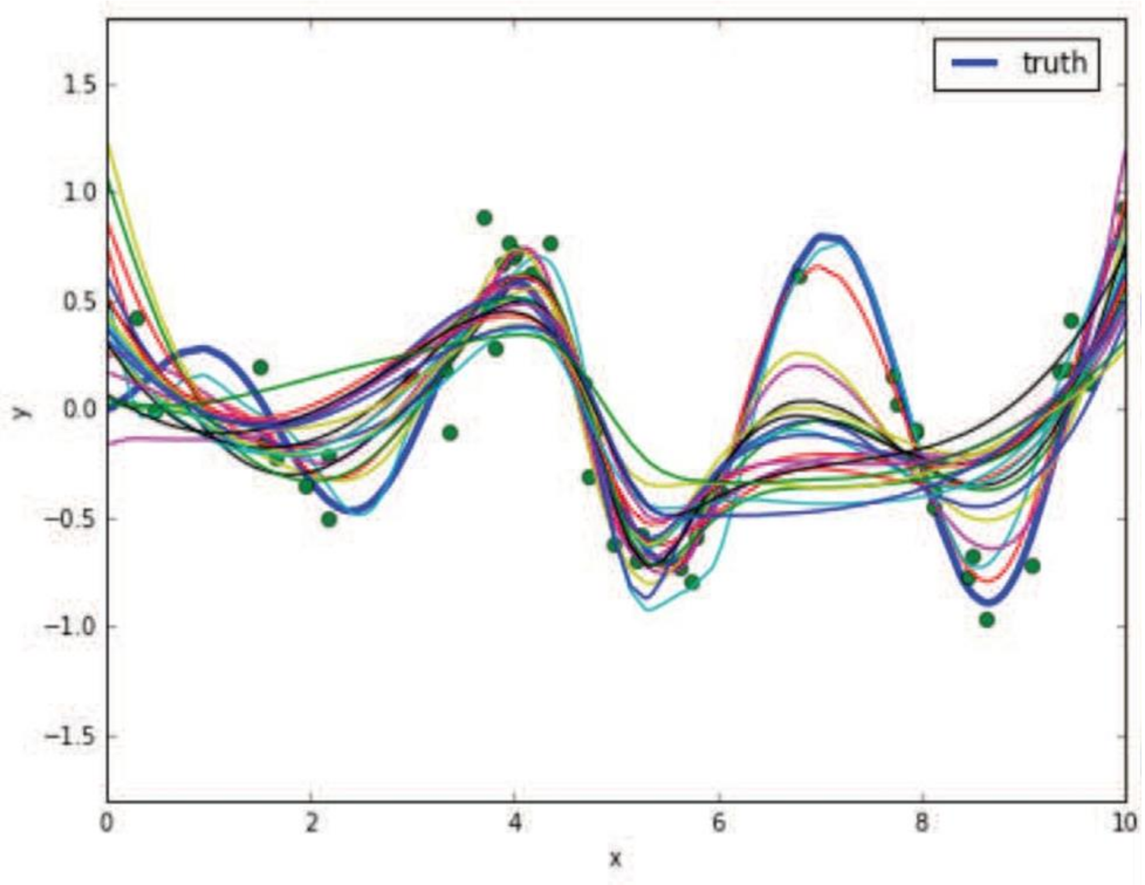
Wolpert and McCready proved:

- if a [learning] algorithm performs well on a certain class of problems then it necessarily pays for that with degraded performance on the set of all remaining problems

There is no universally good machine learning algorithm (when one has finite data)

- Naive Bayesian classification performs well for text classification with smaller data sets
- Linear Support Vector Machines perform well for text classification

Ensembles



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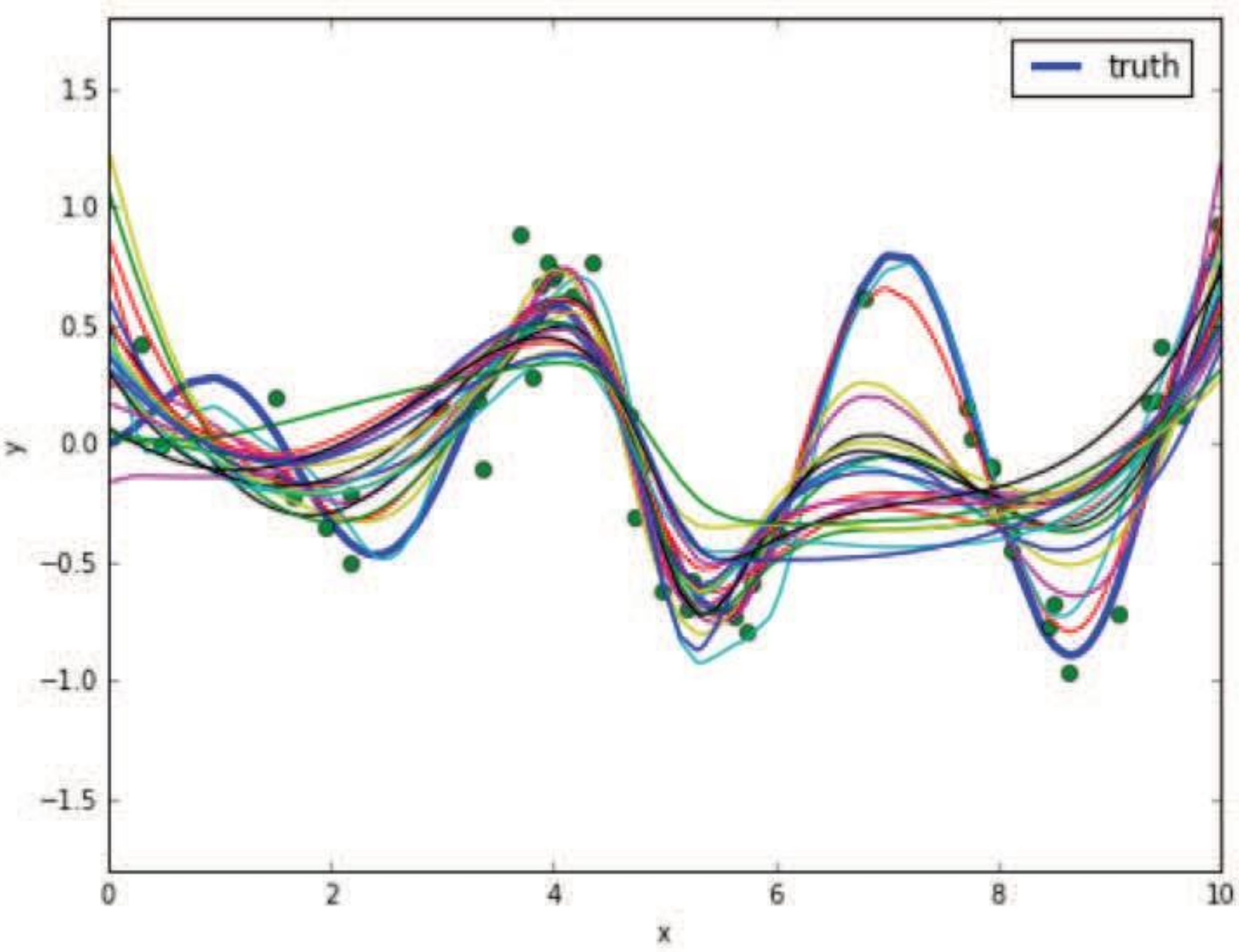
Ensembles

Given only data, we do not know the truth and can only estimate what may be the “truth”

An ensemble is a collection of possible/reasonable models

From this we can understand the **variability** and range of predictions that is realistic

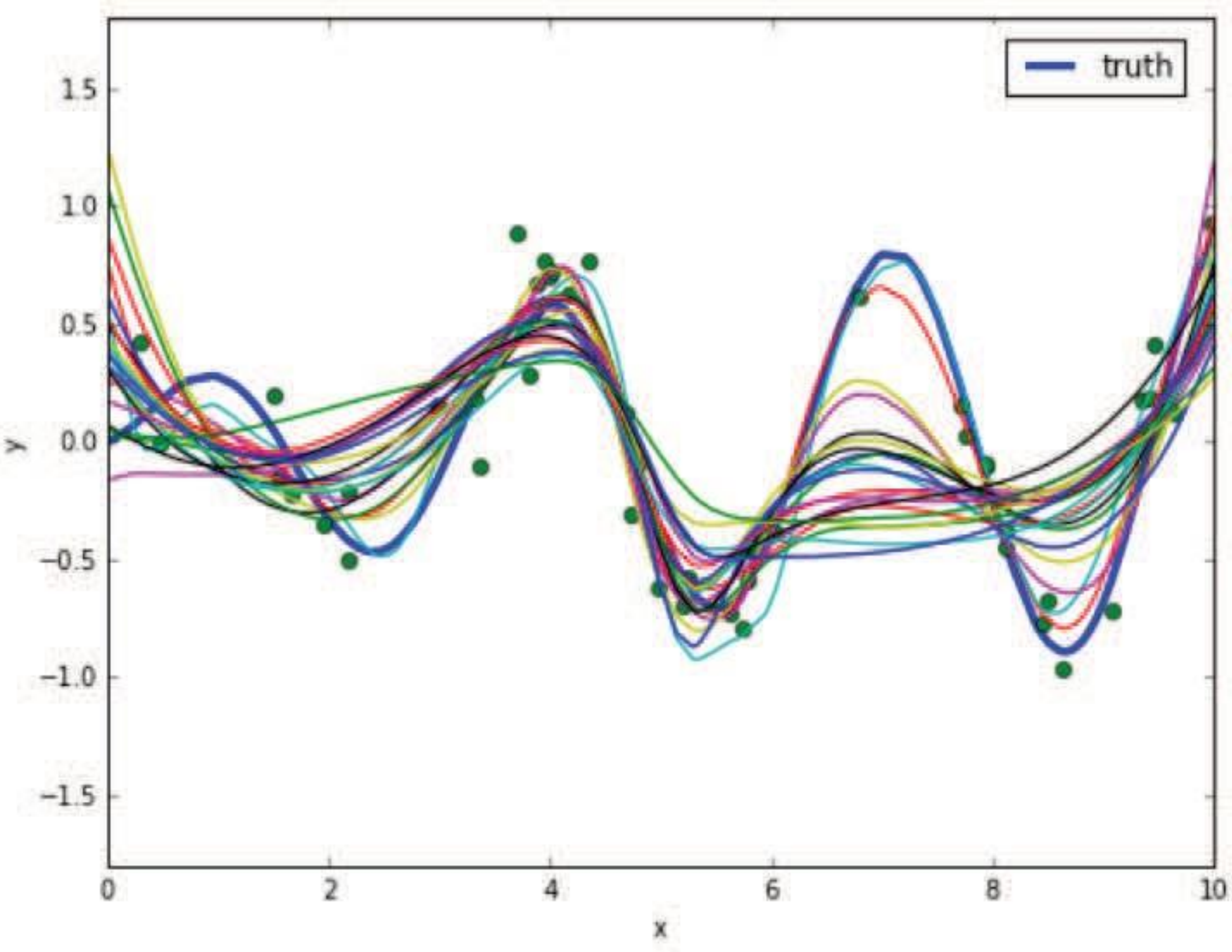


Ensembles

Generating an ensemble is a whole statistical subject in itself

Often we average the predictions over the models in an ensemble to improve performance

$$\hat{y}(x) = \frac{1}{M}\sum_{i=1}^{M} \hat{y}^{(i)}(x)$$



Laboratory in Week 6

Regression in Python, 3 Activities

- Examine the bias of the linear regression model
- Illustrates the fitting of a different type of model
- Illustrates ensembles

Recap: Learning Outcomes

Week 6

By the end of this week you should be able to:

- Fit linear regression and polynomial regression models to a given dataset (in tutorials)
- Explain overfitting and underfitting of different models
- Comprehend bias and variance trade-off
- Comprehend the importance of “No Free Lunch Theorem”
- Explain what ensemble models are

Home Activities

Suggested Activities for the week

You must use **knowledge** about your **data** and the **context** of the world we live in (or the world your data lives in) to select an appropriate machine learning model.

There is no such thing as a single, universally-best machine learning algorithm.

Articles

Read Alex Guanga, “Machine Learning: Bias vs Variance”, becominghuman.ai, October 2018
Read Sydney Firmin, “There is no free lunch in data science”, KDnuggets, September 2019. Summarized in the paragraph “No Free Lunch for Supervised Machine Learning”.

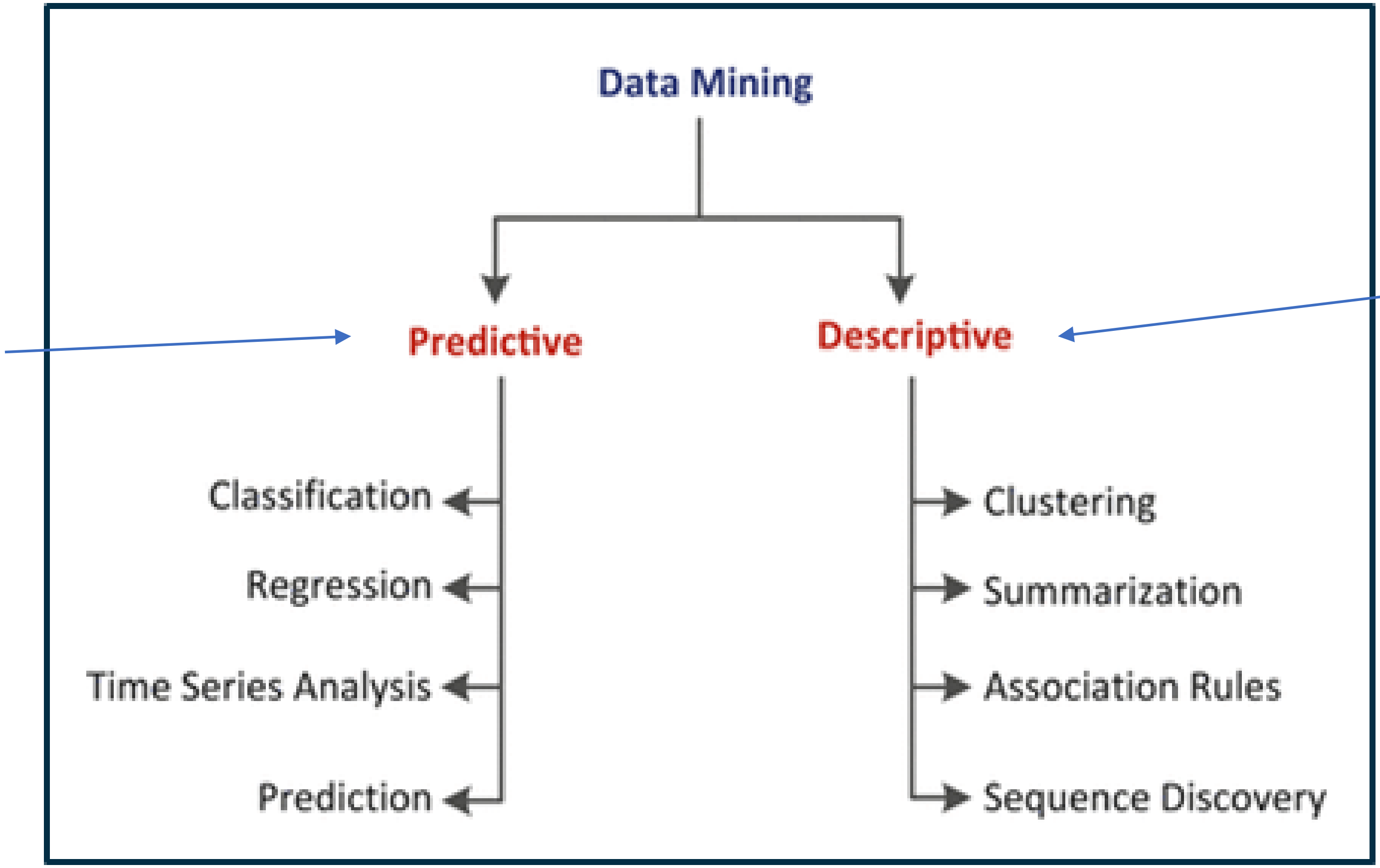
Summary

(So far)

Will be discussed in Forum

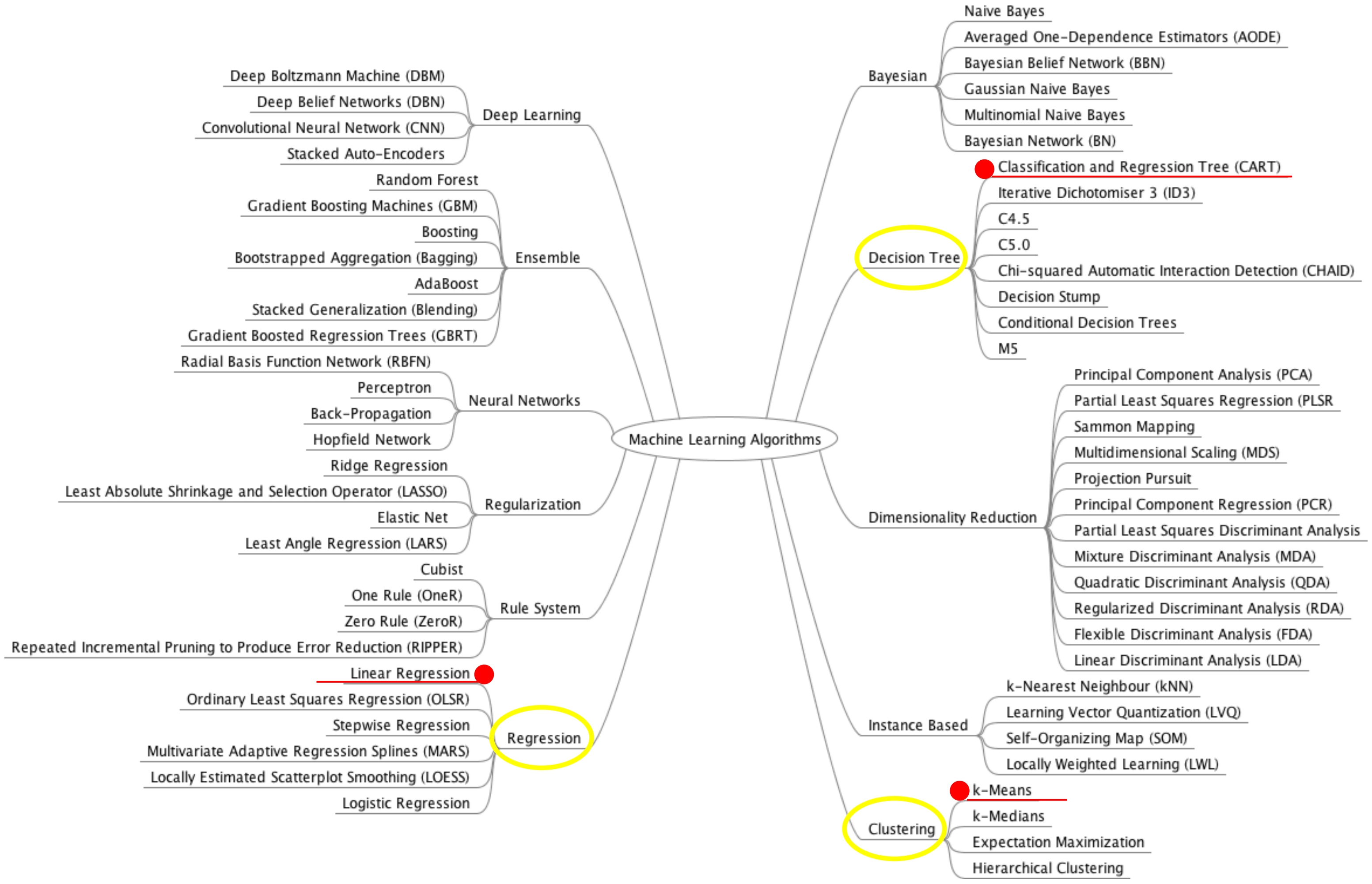
Predictive vs Descriptive

Make prediction using statistical and machine learning techniques



Gain insight from historical data

Machine Learning Algorithms



- Machine Learning Algorithms
  - Deep Learning
    - Deep Boltzmann Machine (DBM)
    - Deep Belief Networks (DBN)
    - Convolutional Neural Network (CNN)
    - Stacked Auto-Encoders
  - Ensemble
    - Random Forest
    - Gradient Boosting Machines (GBM)
    - Boosting
    - Bootstrapped Aggregation (Bagging)
    - AdaBoost
    - Stacked Generalization (Blending)
    - Gradient Boosted Regression Trees (GBRT)
  - Neural Networks
    - Radial Basis Function Network (RBFN)
    - Perceptron
    - Back-Propagation
    - Hopfield Network
  - Regularization
    - Ridge Regression
    - Least Absolute Shrinkage and Selection Operator (LASSO)
    - Elastic Net
    - Least Angle Regression (LARS)
  - Rule System
    - Cubist
    - One Rule (OneR)
    - Zero Rule (ZeroR)
    - Repeated Incremental Pruning to Produce Error Reduction (RIPPER)
  - Regression
    - Linear Regression
    - Ordinary Least Squares Regression (OLSR)
    - Stepwise Regression
    - Multivariate Adaptive Regression Splines (MARS)
    - Locally Estimated Scatterplot Smoothing (LOESS)
    - Logistic Regression
  - Bayesian
    - Naive Bayes
    - Averaged One-Dependence Estimators (AODE)
    - Bayesian Belief Network (BBN)
    - Gaussian Naive Bayes
    - Multinomial Naive Bayes
    - Bayesian Network (BN)
  - Decision Tree
    - Classification and Regression Tree (CART)
    - Iterative Dichotomiser 3 (ID3)
    - C4.5
    - C5.0
    - Chi-squared Automatic Interaction Detection (CHAID)
    - Decision Stump
    - Conditional Decision Trees
    - M5
  - Dimensionality Reduction
    - Principal Component Analysis (PCA)
    - Partial Least Squares Regression (PLSR
    - Sammon Mapping
    - Multidimensional Scaling (MDS)
    - Projection Pursuit
    - Principal Component Regression (PCR)
    - Partial Least Squares Discriminant Analysis
    - Mixture Discriminant Analysis (MDA)
    - Quadratic Discriminant Analysis (QDA)
    - Regularized Discriminant Analysis (RDA)
    - Flexible Discriminant Analysis (FDA)
    - Linear Discriminant Analysis (LDA)
  - Instance Based
    - k-Nearest Neighbour (kNN)
    - Learning Vector Quantization (LVQ)
    - Self-Organizing Map (SOM)
    - Locally Weighted Learning (LWL)
  - Clustering
    - k-Means
    - k-Medians
    - Expectation Maximization
    - Hierarchical Clustering