Introduction to Machine Learning

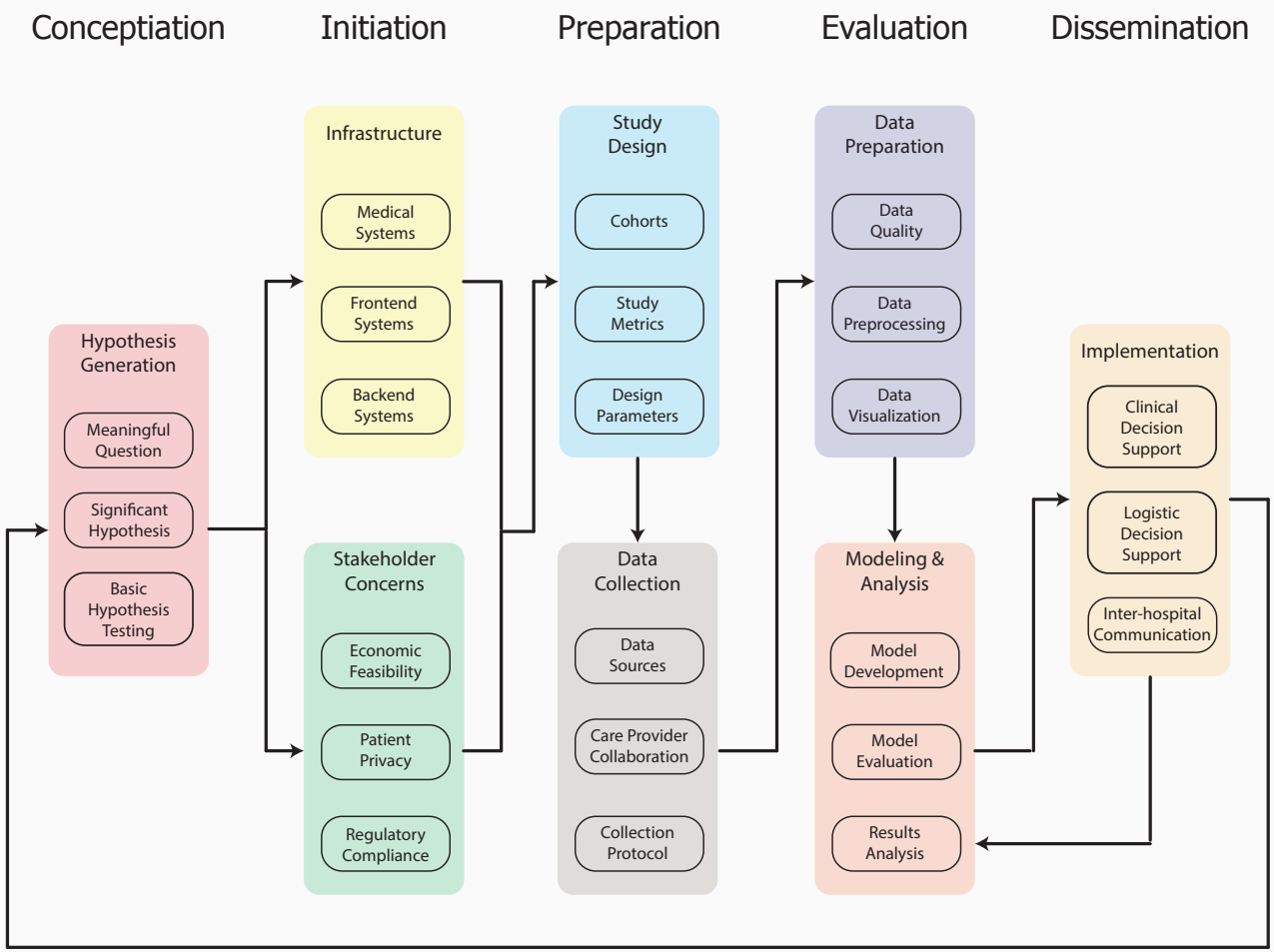
Digital Transformation of Healthcare

Michoel Snow M.D. Ph.D. and Glen Ferguson Ph.D.

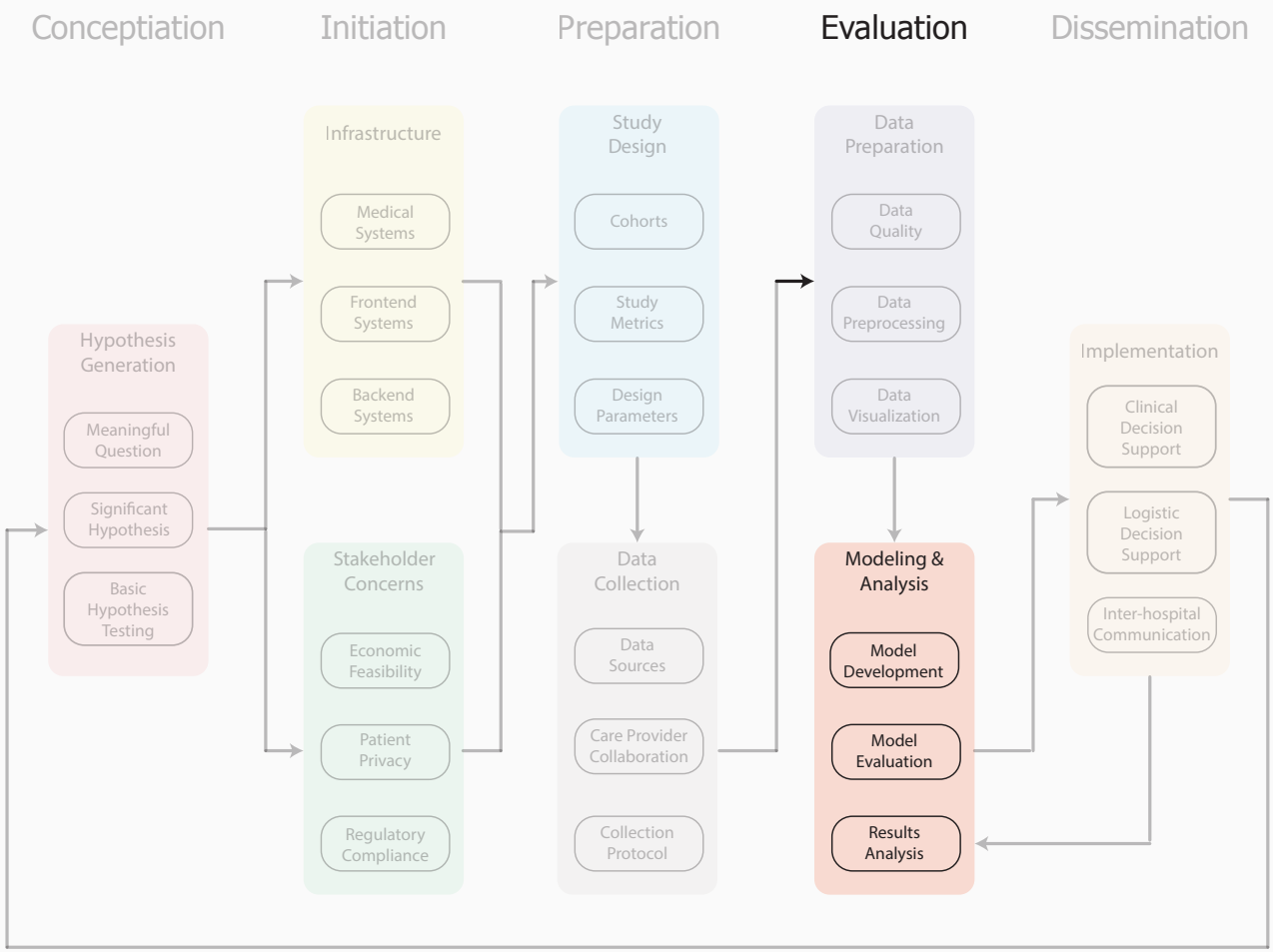
Center for Health Data Innovations

Intro to Machine Learning

Bioinformatics Pipeline



Data Analysis

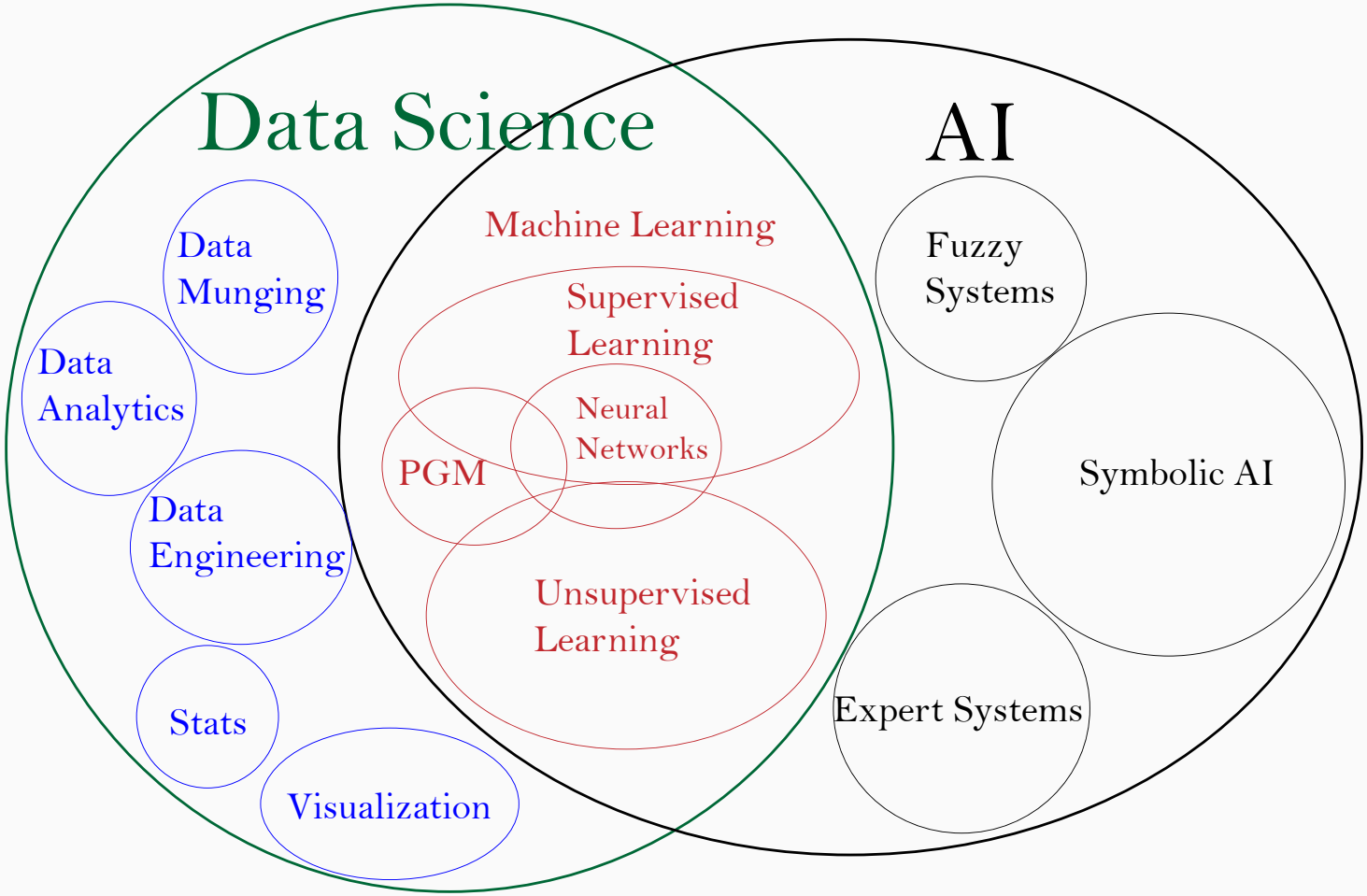


Machine Learning

What is machine learning?

What is Machine Learning?

Machine Learning is part of multiple overlapping disciplines and is often associated with both Data Science and Artificial intelligence.



What is Machine Learning?

Machine learning is a discipline in AI where algorithms use data to improve a model

What is Machine Learning?

Machine learning is a discipline in AI where algorithms use data to improve a model

- Algorithm is a specification of how to solve a problem

What is Machine Learning?

Machine learning is a discipline in AI where algorithms use data to improve a model

- Algorithm is a specification of how to solve a problem
- Data is information about the problem we are trying to solve

What is Machine Learning?

Machine learning is a discipline in AI where algorithms use data to improve a model

- Algorithm is a specification of how to solve a problem
- Data is information about the problem we are trying to solve
- Model

What is Machine Learning?

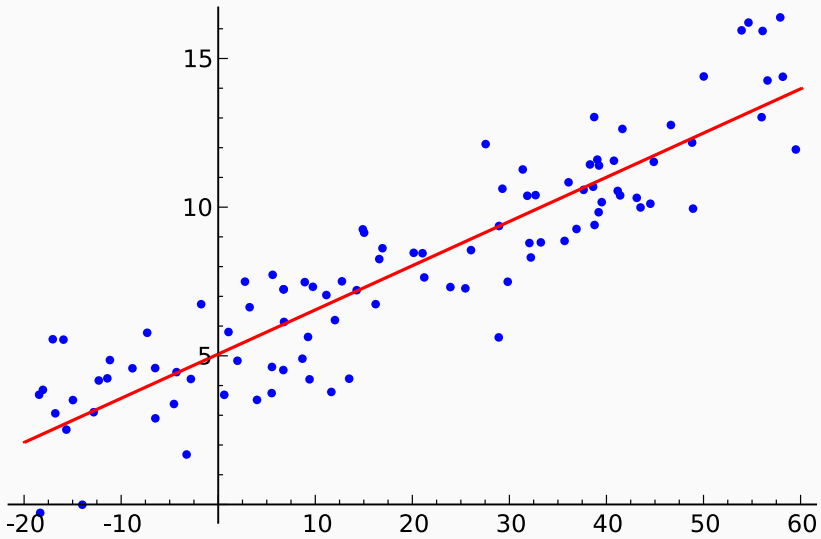
Machine learning is a discipline in AI where algorithms use data to improve a model

- Algorithm is a specification of how to solve a problem
- Data is information about the problem we are trying to solve
- Model
    - Scientific - a simplified and idealized understanding of physical systems

What is Machine Learning?

Machine learning is a discipline in AI where algorithms use data to improve a model

- Algorithm is a specification of how to solve a problem
- Data is information about the problem we are trying to solve
- Model
  - Scientific - a simplified and idealized understanding of physical systems
  - Computer Science - a simulation to reproduce the behavior of a system



What is Machine Learning?

- Machine learning is a discipline that uses data to improve a model
  - Algorithm Examples
    - Logistic Regression
    - Random Forest
    - Neural Networks

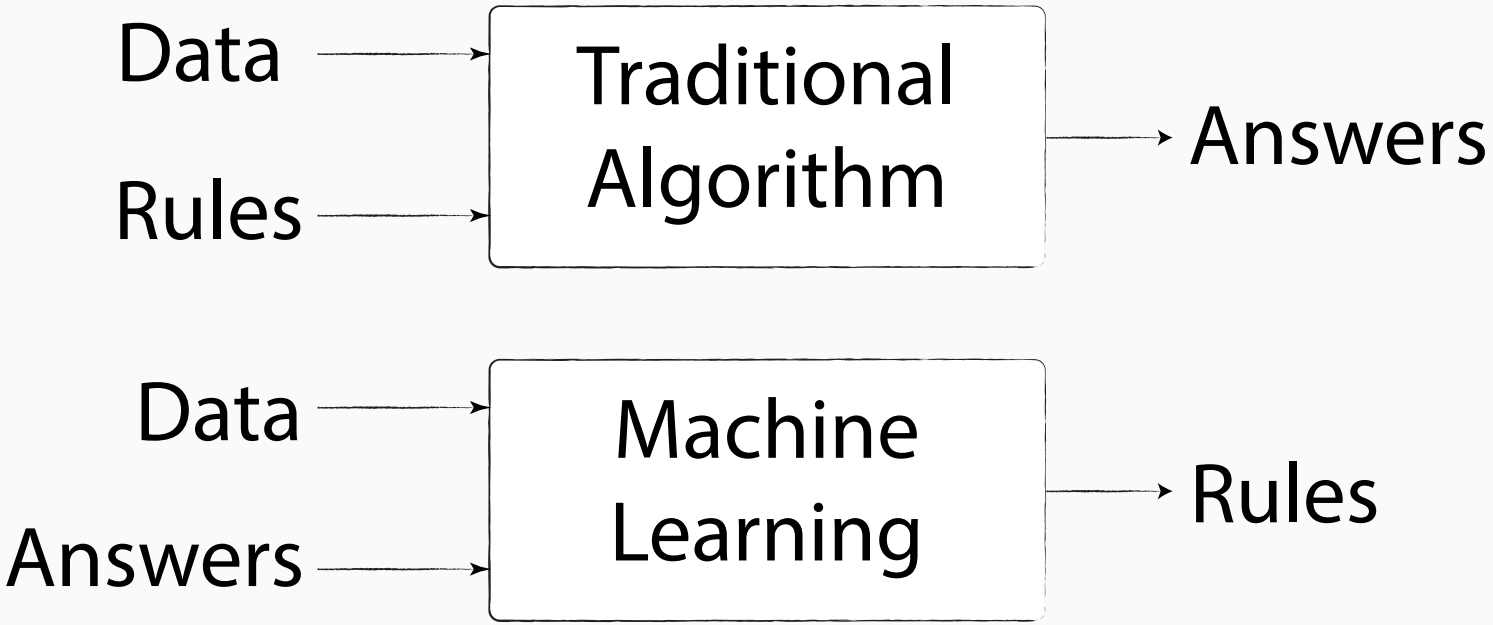
What is Machine Learning?

- Machine learning is a discipline that uses data to improve a model
  - Algorithm Examples
    - Logistic Regression
    - Random Forest
    - Neural Networks
- Machine learning contains multiple classes of learning algorithms
  - Supervised Learning
  - Unsupervised Learning
  - Reinforcement Learning

What is Machine Learning?

- Machine learning is a discipline that uses data to improve a model
  - Algorithm Examples
    - Logistic Regression
    - Random Forest
    - Neural Networks
- Machine learning contains multiple classes of learning algorithms
  - Supervised Learning
  - Unsupervised Learning
  - Reinforcement Learning
- Machine learning models perform tasks, such as language translation and identifying objects, that present extraordinary difficulty for standard algorithms
  - ImageNet Large Scale Visual Recognition Challenge

Traditional Programming vs. Machine Learning



Types of Learning

- Supervised Learning
  - Prediction of specific value for given data
    - Algorithm learns the values (labels) from the data
    - Learning requires the data to the desired prediction
    - Inference is prediction of these labels from *new* data

Types of Learning

- Supervised Learning
  - Prediction of specific value for given data
    - Algorithm learns the values (labels) from the data
    - Learning requires the data to the desired prediction
    - Inference is prediction of these labels from *new* data
- Unsupervised Learning
  - Understanding the structure of the data
    - Algorithm learns the structure from the data
    - Learning/inference requires only the data

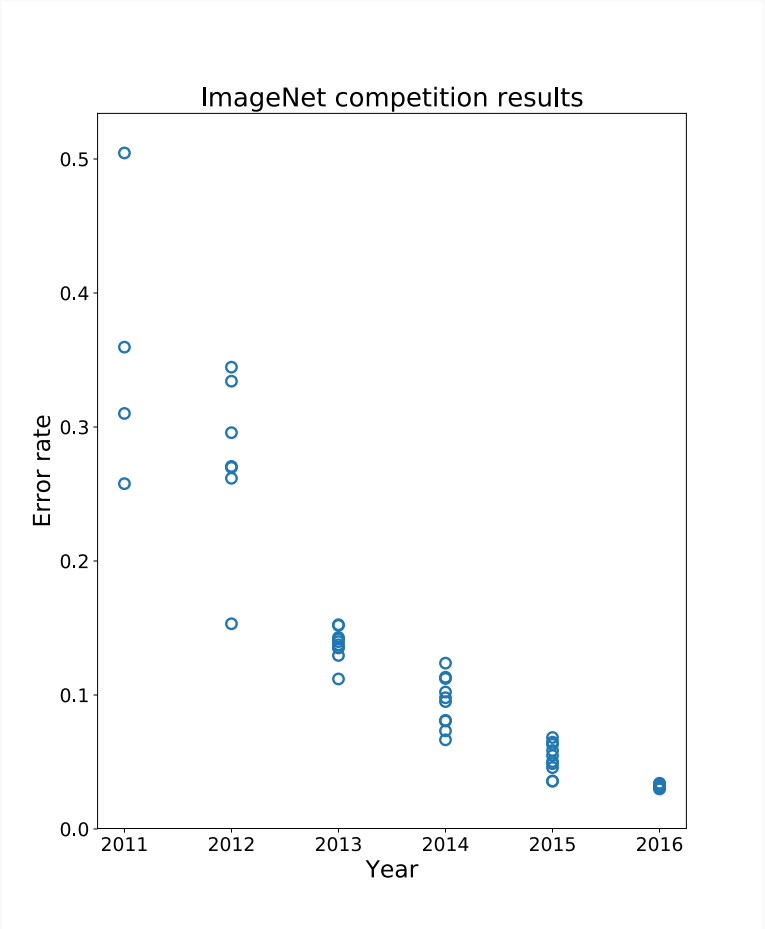
Types of Learning

- Supervised Learning
  - Prediction of specific value for given data
    - Algorithm learns the values (labels) from the data
    - Learning requires the data to the desired prediction
    - Inference is prediction of these labels from *new* data
- Unsupervised Learning
  - Understanding the structure of the data
    - Algorithm learns the structure from the data
    - Learning/inference requires only the data
- Reinforcement Learning
  - Predicting optimal actions for the environment based on rewards
    - Algorithm learns the actions that maximize a reward for an environment
    - Learning requires information about the environment, rewards and actions
    - Inference is prediction of optimal actions actions for environment

What is Machine Learning?

- ImageNet Large Scale Visual Recognition Challenge
  - Algorithmic recognition of 1000 items in 150,000 photos

Figure 1: ImageNet Competition Results,



What is Machine Learning?

- Exercise
  - Using your domain expertise answer the following

What is Machine Learning?

- Exercise
  - Using your domain expertise answer the following
  - Determine two problems in both Supervised and Unsupervised Learning

What is Machine Learning?

- Exercise
  - Using your domain expertise answer the following
  - Determine two problems in both Supervised and Unsupervised Learning
  - What types of data are required for each?

What is Machine Learning?

- Exercise
  - Using your domain expertise answer the following
  - Determine two problems in both Supervised and Unsupervised Learning
  - What types of data are required for each?
  - How does ML fit into the overall health care informatics pipeline?

What is Machine Learning?

- Exercise
  - Using your domain expertise answer the following
  - Determine two problems in both Supervised and Unsupervised Learning
  - What types of data are required for each?
  - How does ML fit into the overall health care informatics pipeline?
  - How can you used both in a single project?

Supervised Learning

Types of Supervised Learning

What are the type of supervised learning?

- Regression - predicting a continuous numerical value

Types of Supervised Learning

What are the type of supervised learning?

- Regression - predicting a continuous numerical value
- Classification - prediction of discreet class labels

Types of Supervised Learning

What are the type of supervised learning?

- Regression - predicting a continuous numerical value
- Classification - prediction of discreet class labels

Figure 2: Non-linear Regression, By Alexeicolin - Own work, CC BY-SA 3.0

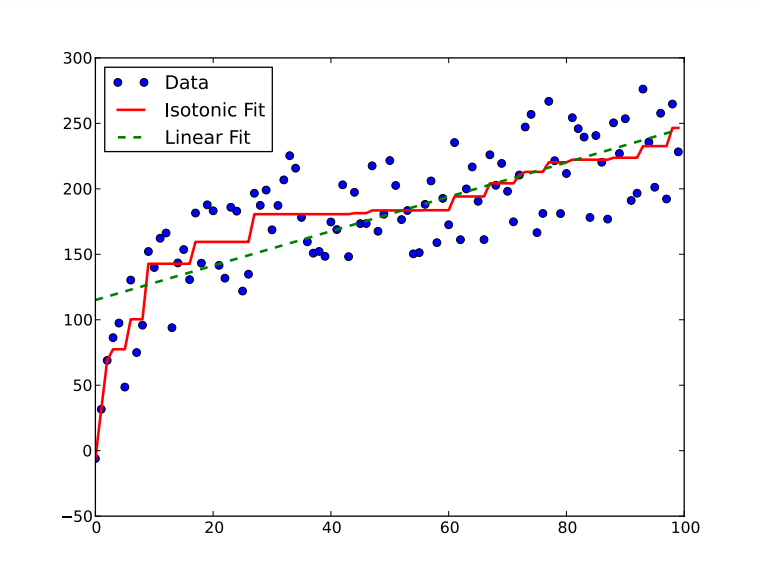
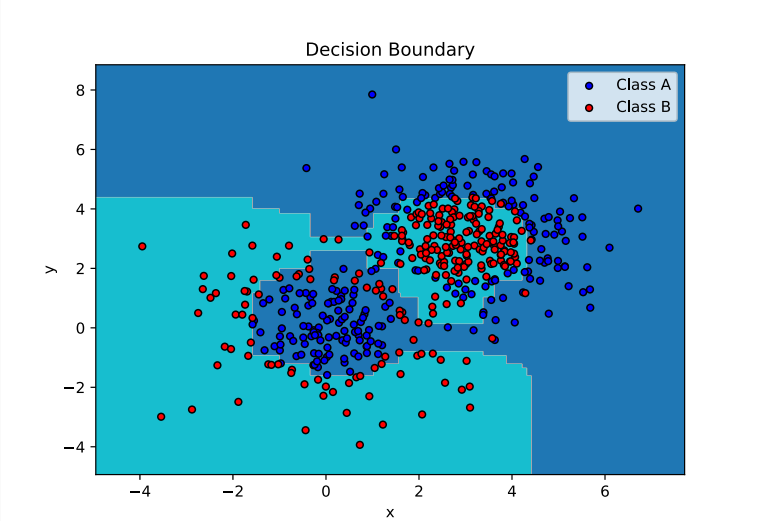


Figure 3: Classification, By Alisneaky Own work, CC BY-SA 4.0



Types of Predictions

- Exercise
  - Determine the types of predictions for the Supervised Learning problem above

Types of Predictions

- Exercise
  - Determine the types of predictions for the Supervised Learning problem above
  - How many classes do the Classifications problems have?

Basic Methods

Linear and Logistic Regression

- Linear Regression - Predicting continuous values from linearly separable data

Basic Methods

Linear and Logistic Regression

- Linear Regression - Predicting continuous values from linearly separable data
- Logistic Regression - Subclass of Generalized Linear Models for binary class prediction

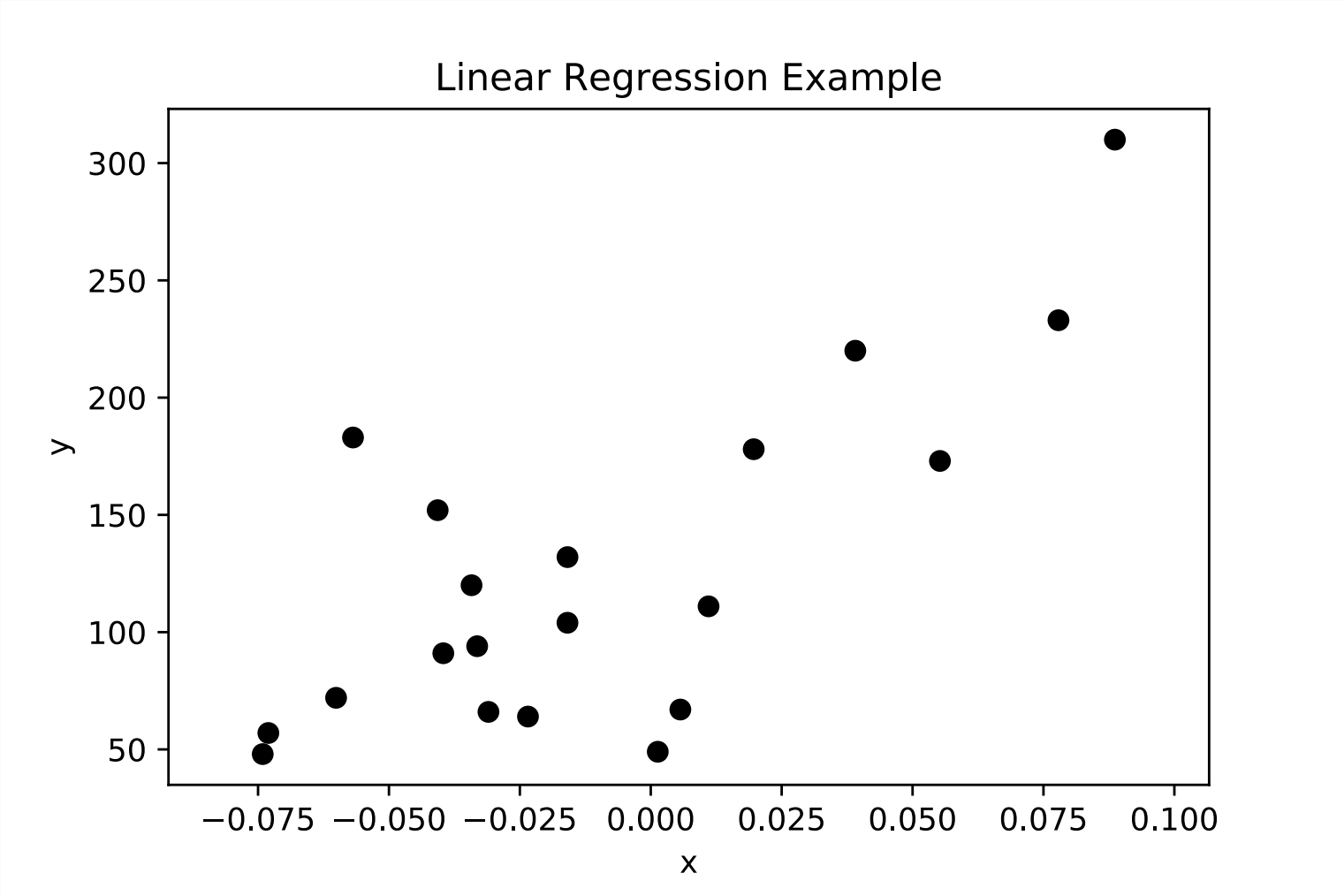
Basic Methods

Linear and Logistic Regression

- Linear Regression - Predicting continuous values from linearly separable data
- Logistic Regression - Subclass of Generalized Linear Models for binary class prediction
- *Data should be linearly separable or variables linearly correlated*

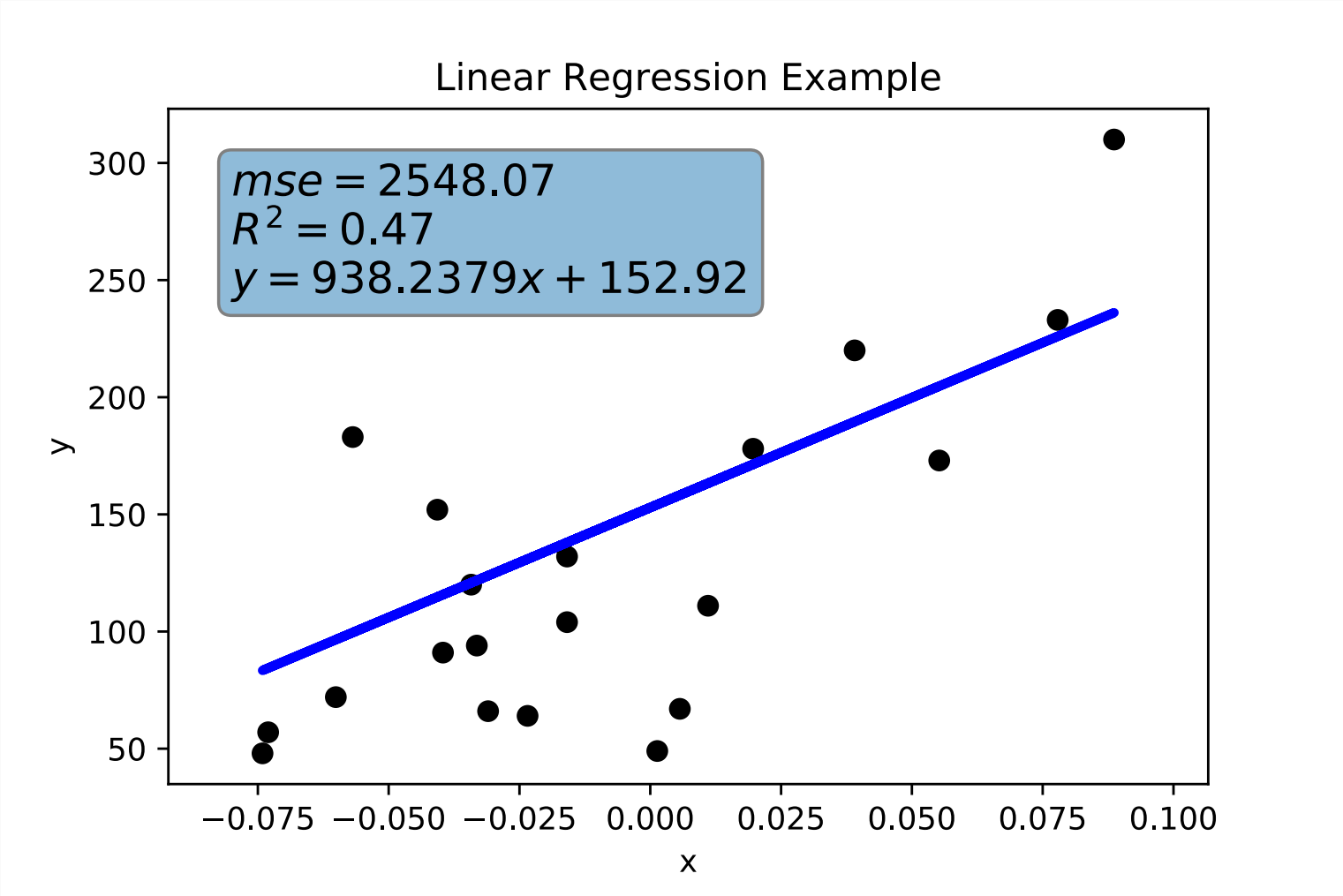
Linear Regression

Predicting continuous values



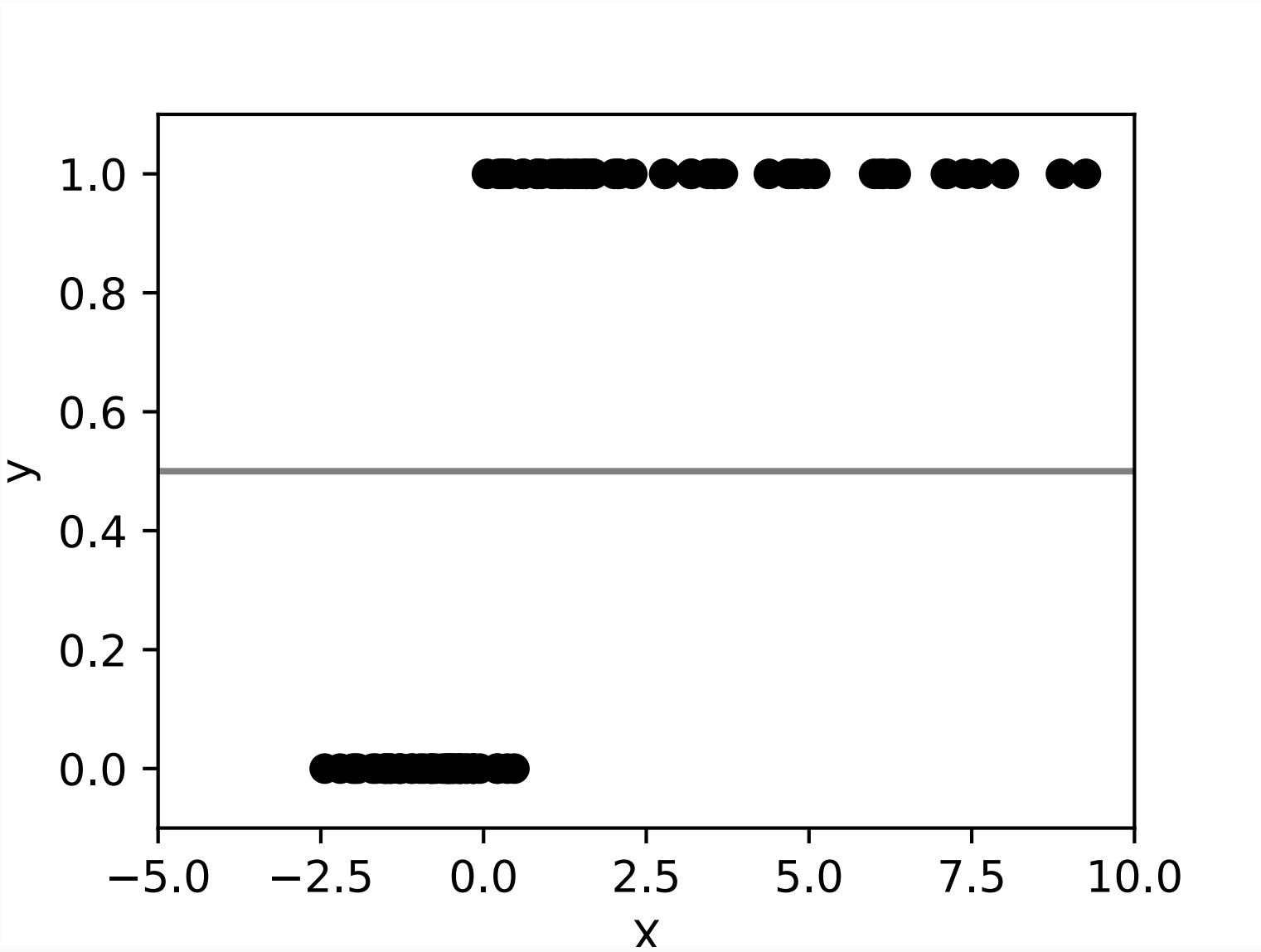
Linear Regression

Predicting continuous values



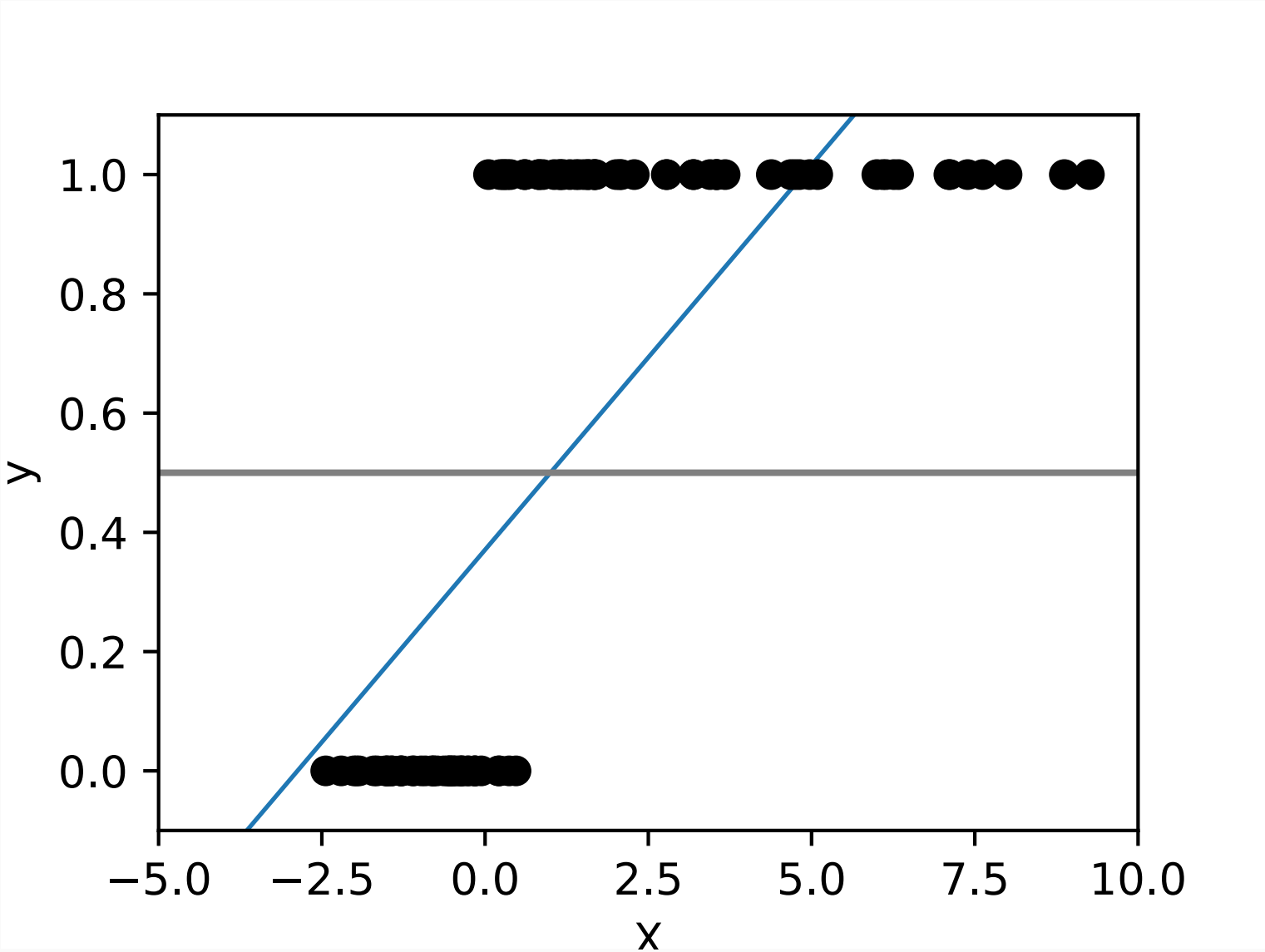
Logistic Regression

What if the data is binary?



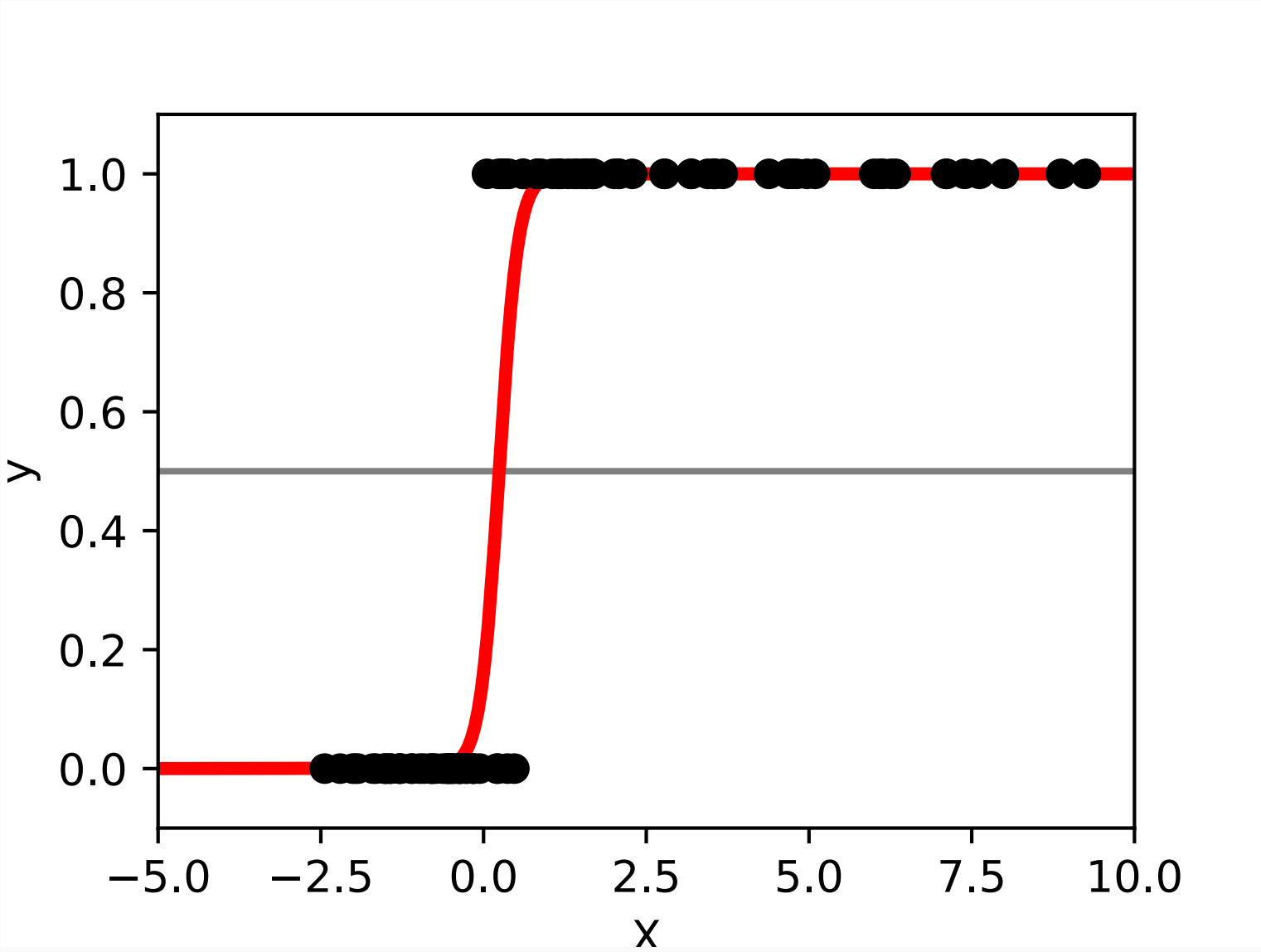
Logistic Regression

The linear fit does not work



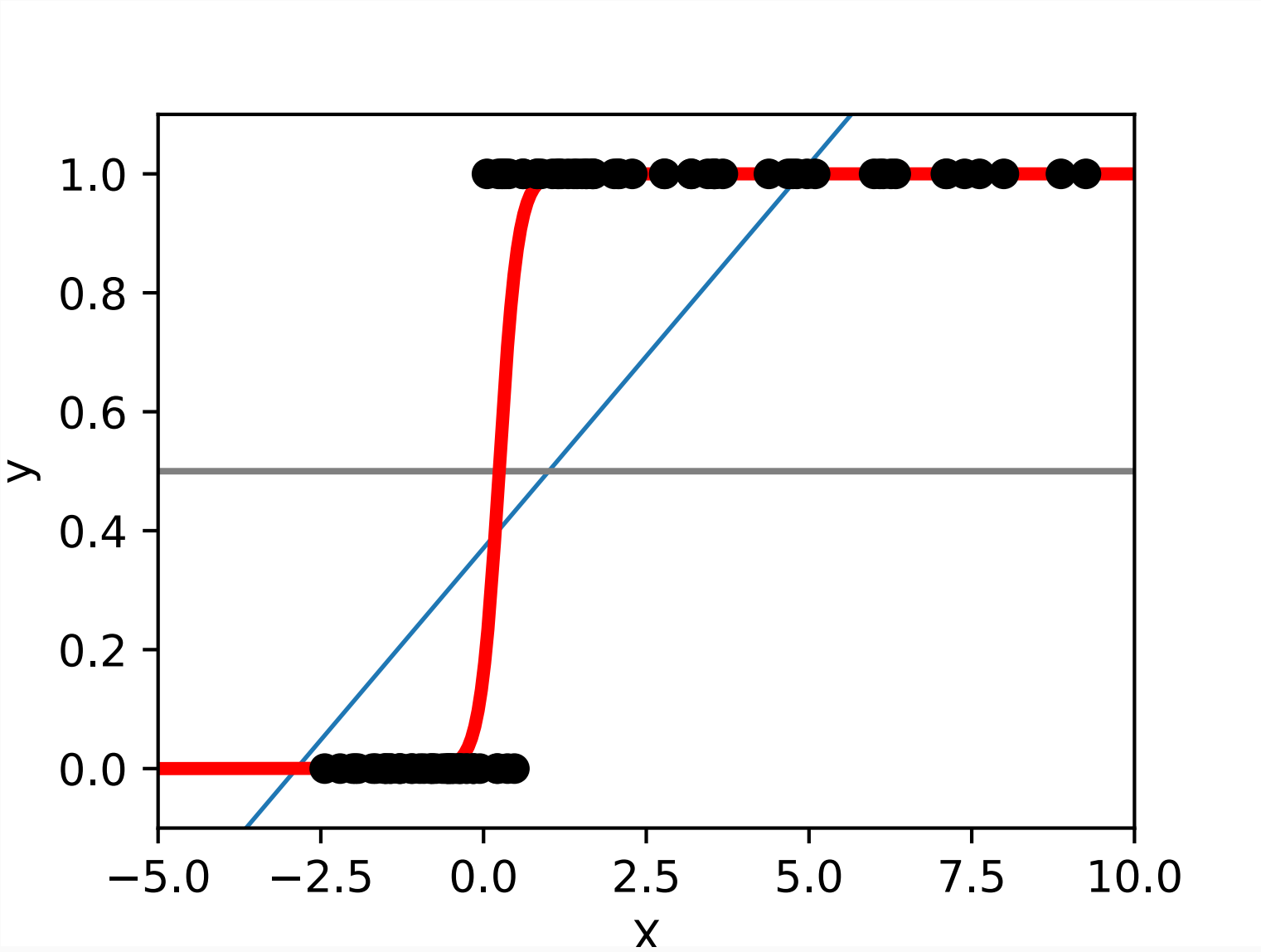
Logistic Regression

Sigmoid function fits the data well



Logistic Regression

Logistic regression fits uses a linear fit to a sigmoid function



Iris Data

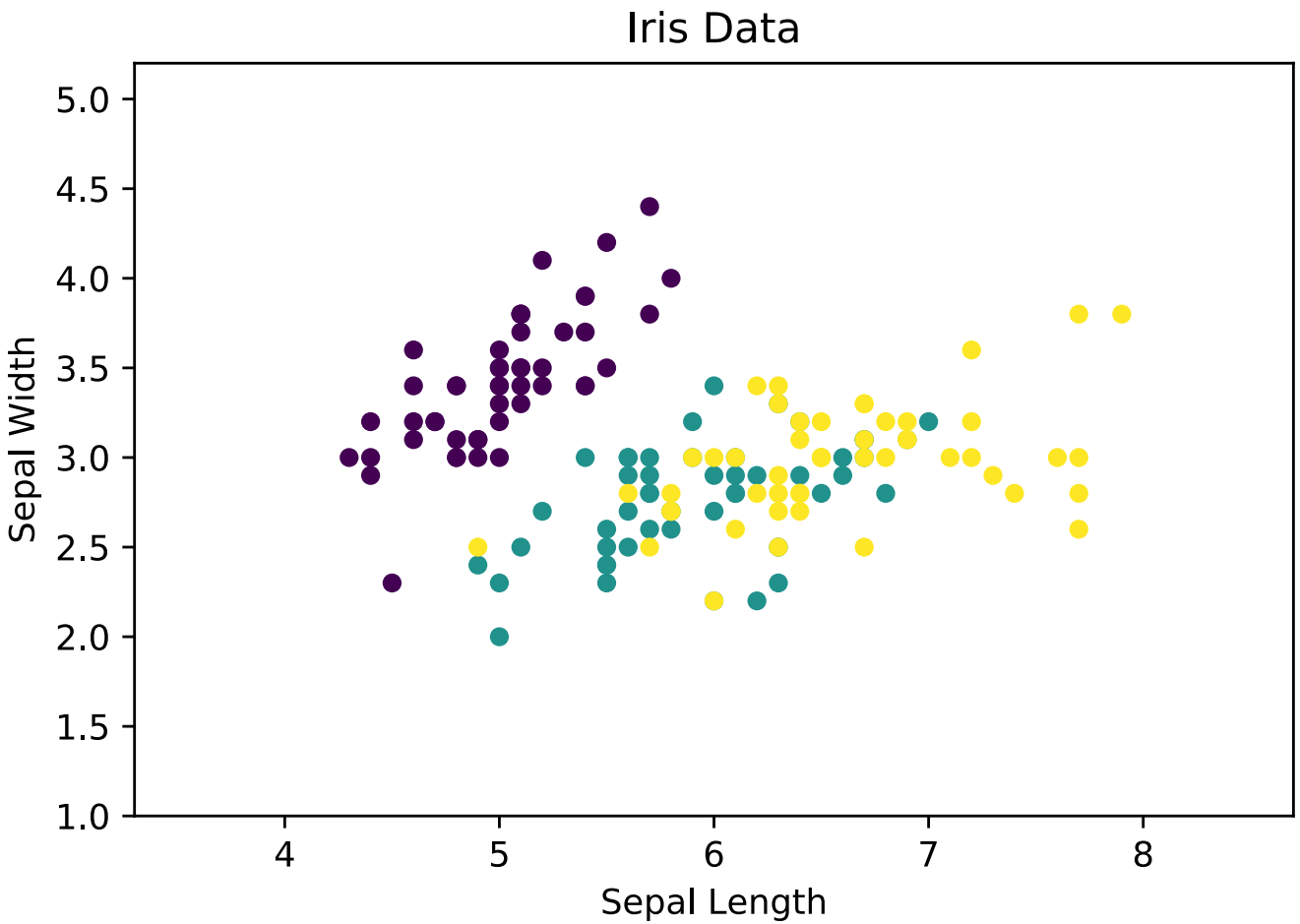
The iris data set is commonly used for teaching machine learning

- Data from 1930's to identify flowers from petal and sepal measurements
- Three species of iris flowers: Setosa, Versicolor and Virginica
- Only a few variables, Sepal width, Sepal length, Petal width and Petal length
- 150 sets of measurements

Figure 4: Versicolor Iris flower, sepal labeled

Iris Data

Dataset of Iris Flower Types



Non-parametric Methods

Support Vector Machines and Decision Trees

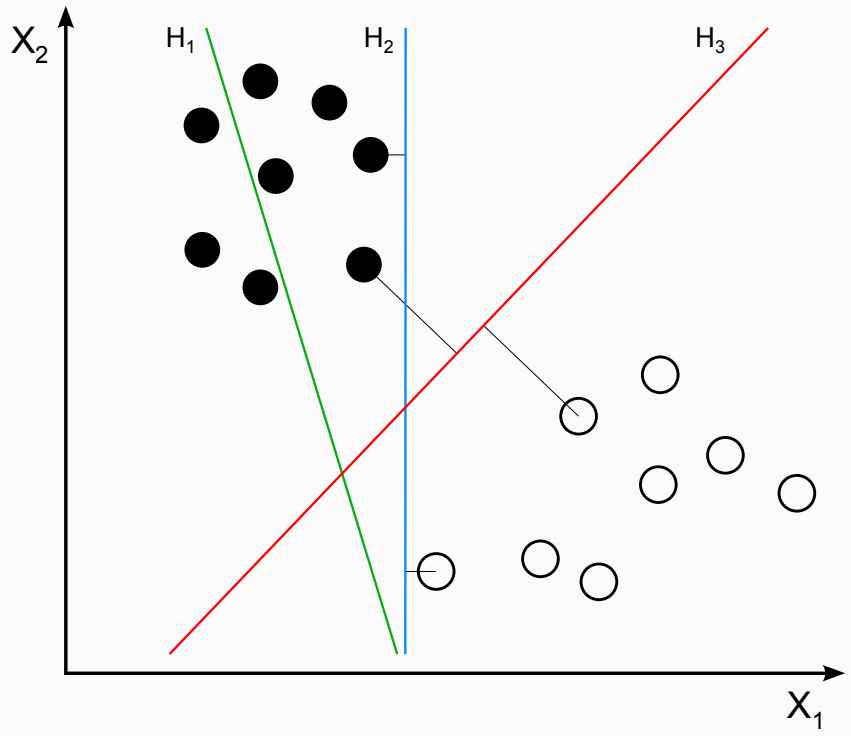
- Support Vector Machine - Prediction by finding the best (hyper)planes that separate the data
- Tree-Based Method - Prediction of using decision-trees
  - Decision Trees
  - Random Forest
  - Boosted Trees

Support Vector Machines

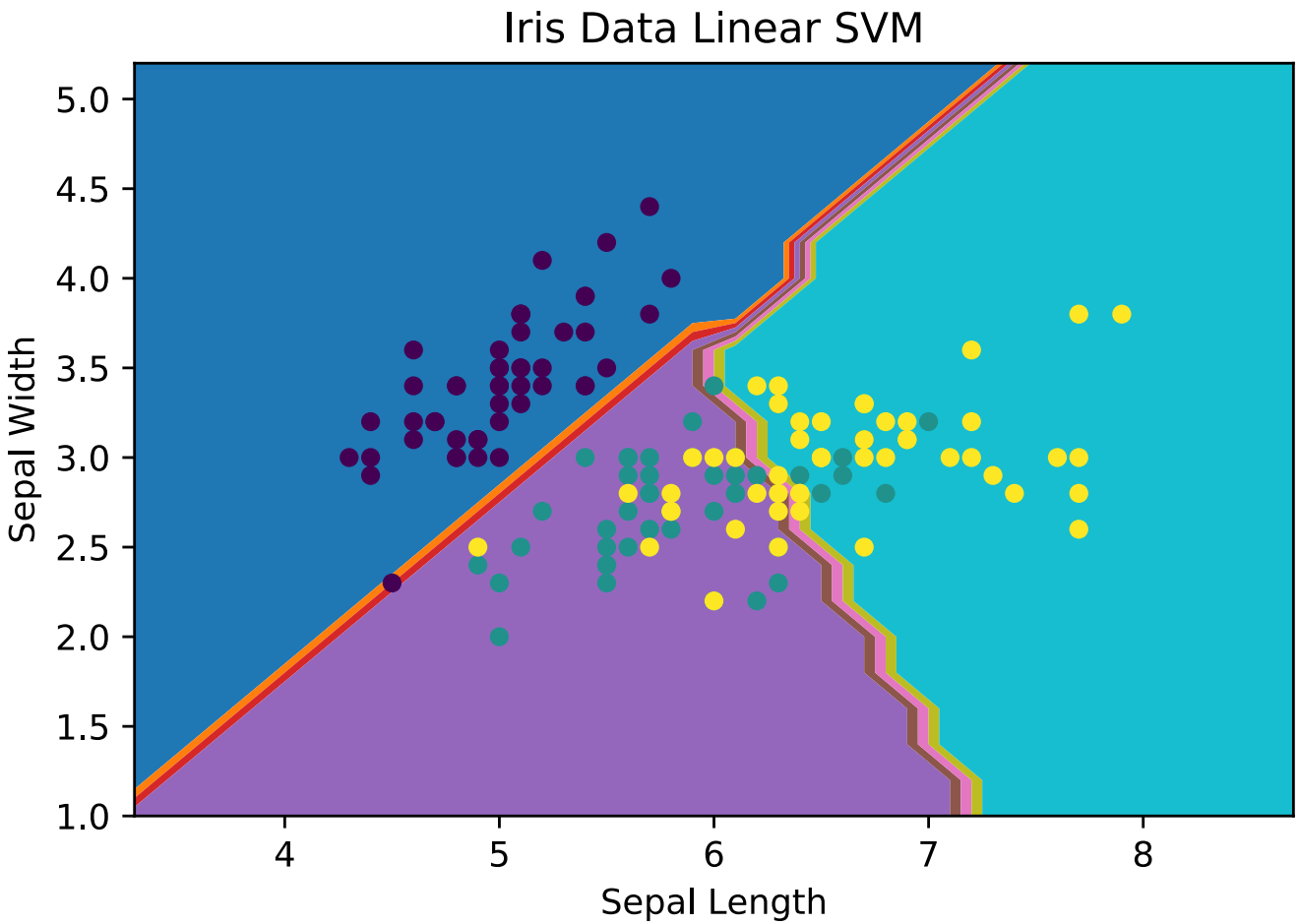
SVC and SVR are a common methods of fitting data

- Finds the plane that *best* divides the data
- Can fit highly non-linear data
- Kernels allow for flexibility but must be chosen by the user
- Does not fit data with more than two classes
- Does not give class probabilities just class membership
- Parameters can be difficult to choose

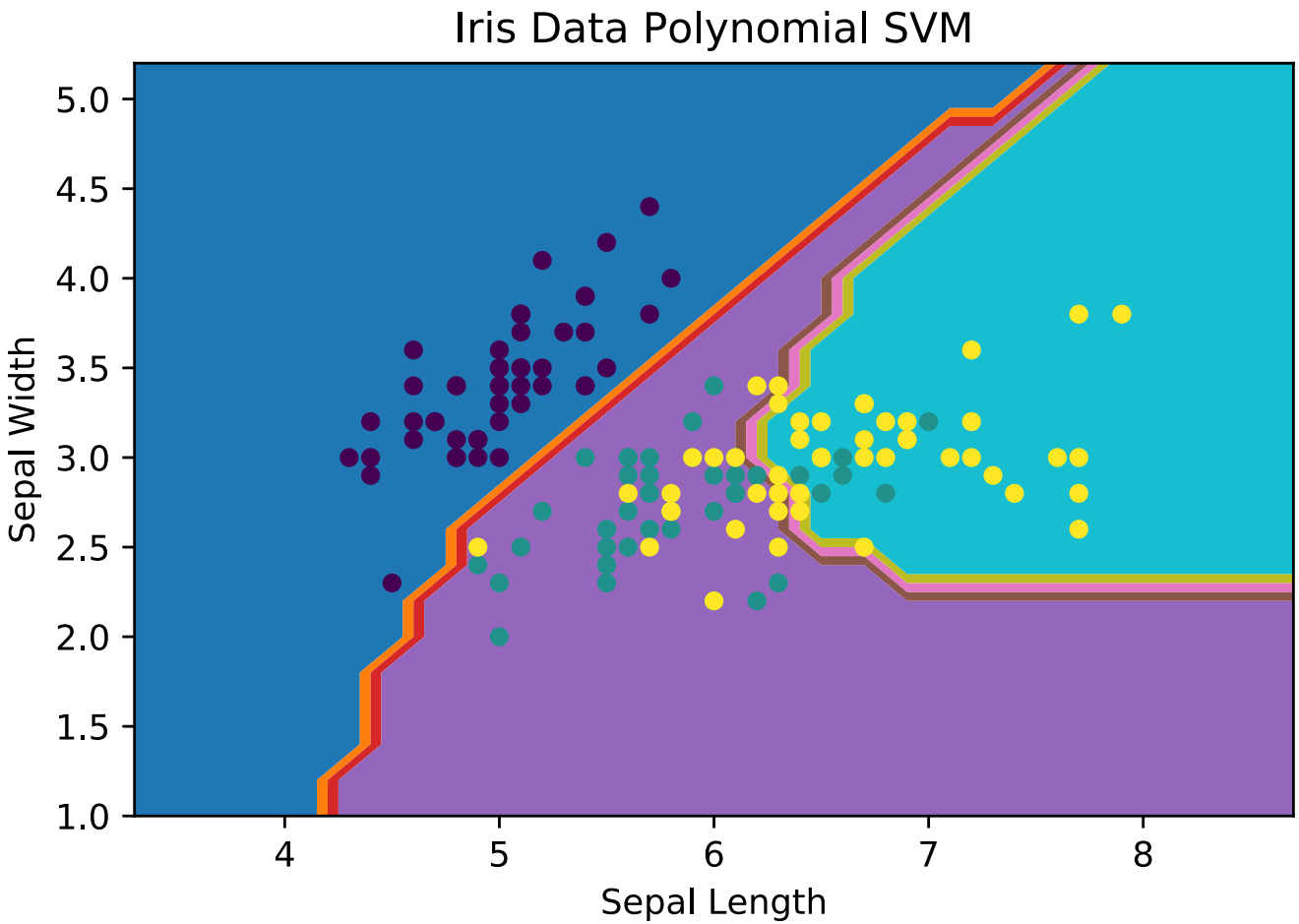
Figure 5: Best plane example, By User:ZackWeinberg, based on PNG by User:Cyc derived from: Svm separating hyperplanes.png, CC BY-SA 3.0



Support Vector Machine



Support Vector Machine

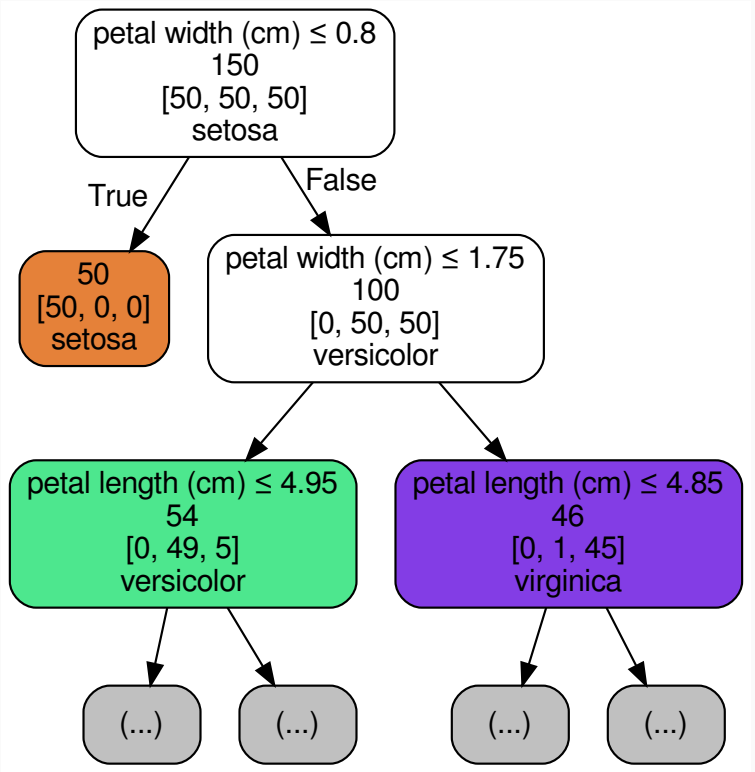


Tree-based Methods

Methods using decision trees or ensembles of decision trees for classification and regression problems

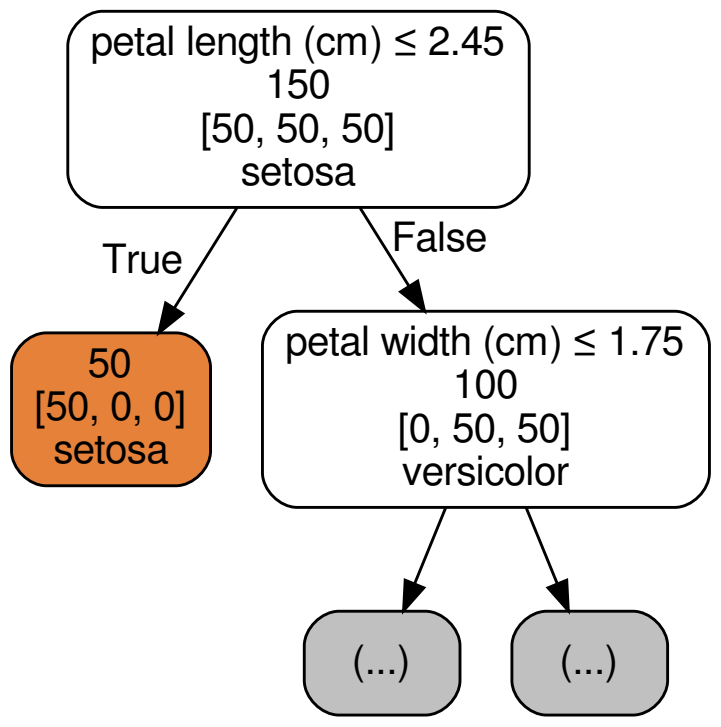
- Fits a decision tree based on the data to predict results
- Can fit highly non-linear data with *high* accuracy
- Models can be very large
- Some models, Random Forest, do not fit sparse data well
- Other models, Boosting, have many parameters that can be difficult to choose

Figure 6: Decision Tree Example

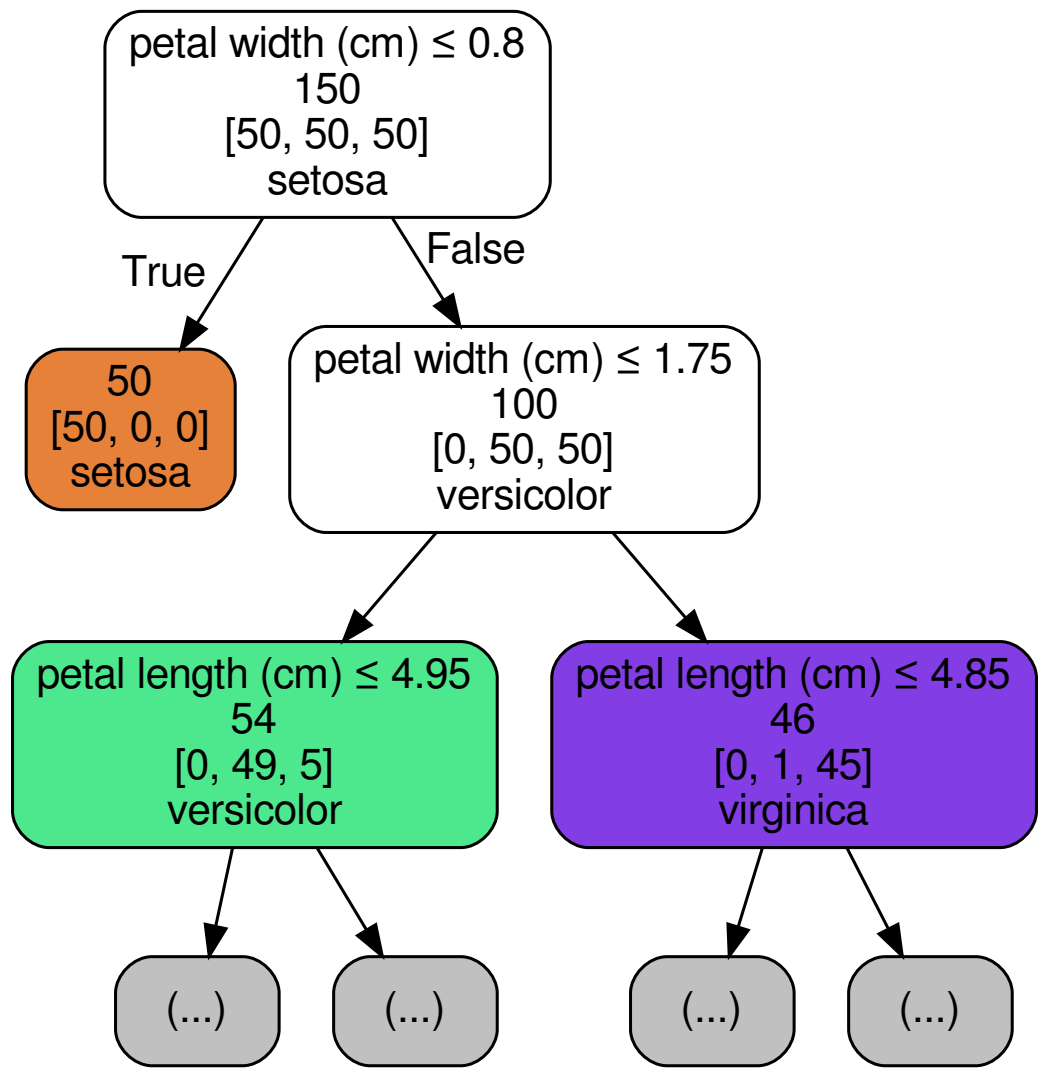


Building a Decision Tree

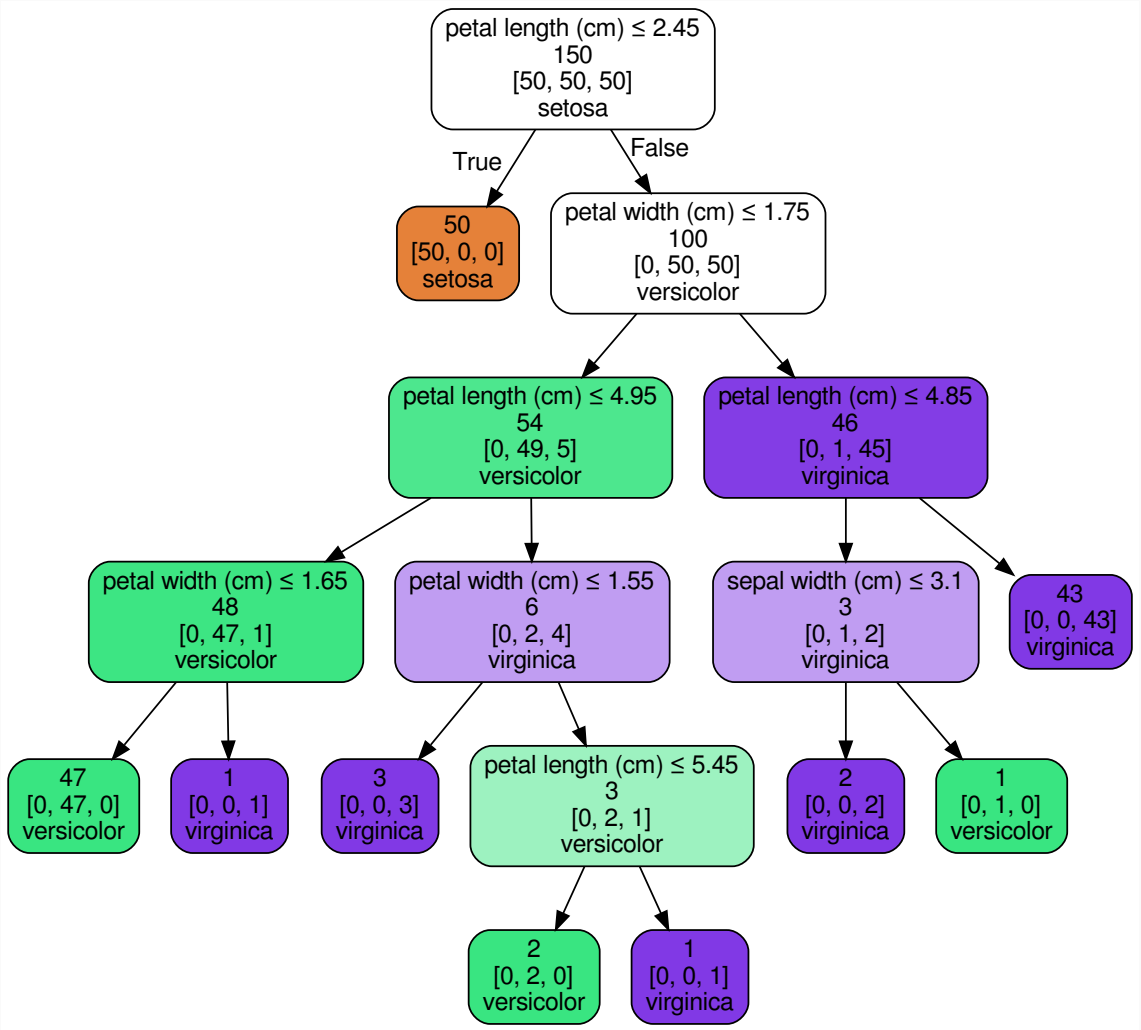
Make splits in the data in such a way that it separates the classes or that minimizes the distance between the predictions in a region.



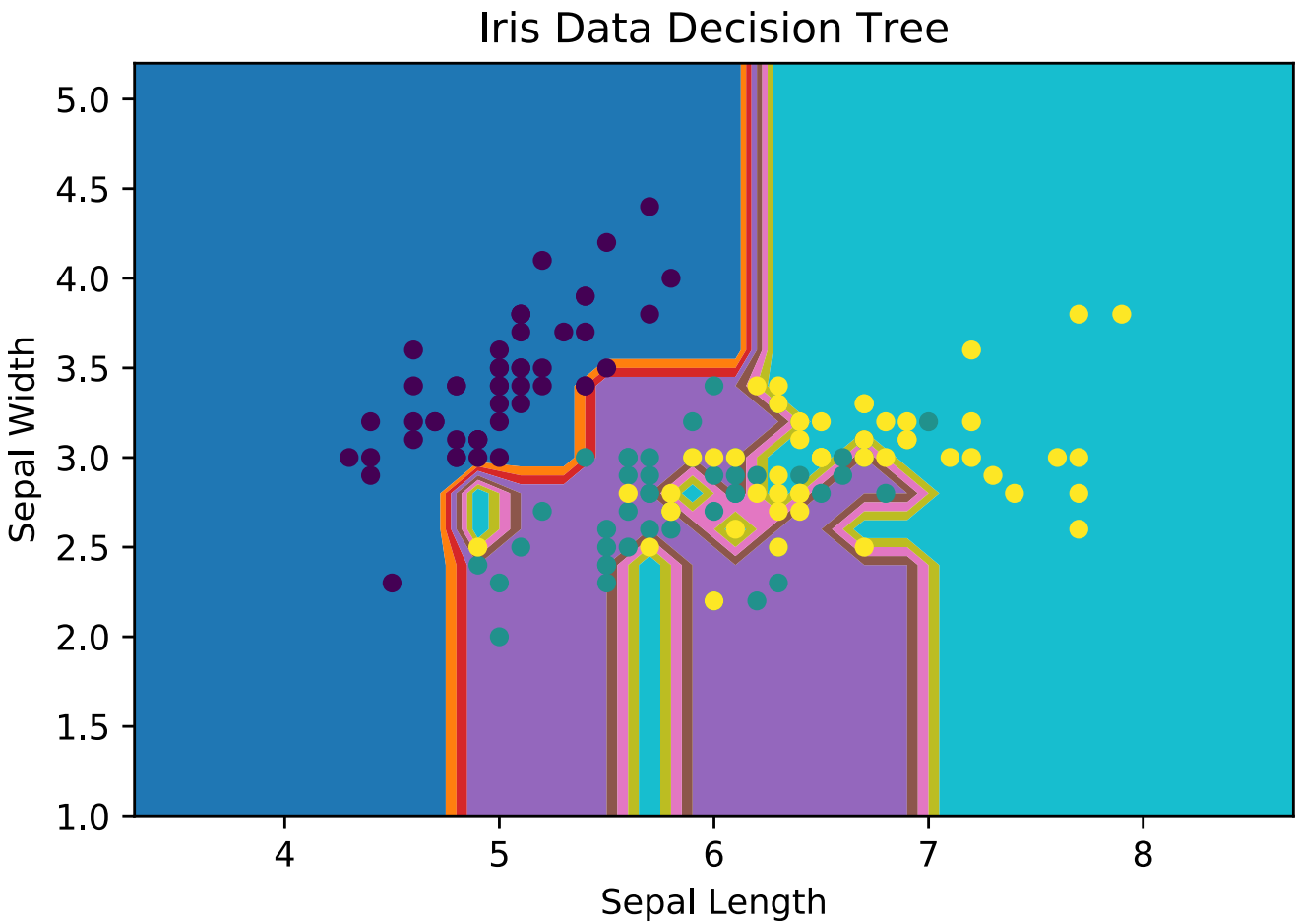
Building a Decision Tree



Building a Decision Tree



Decision Tree Decision Boundary



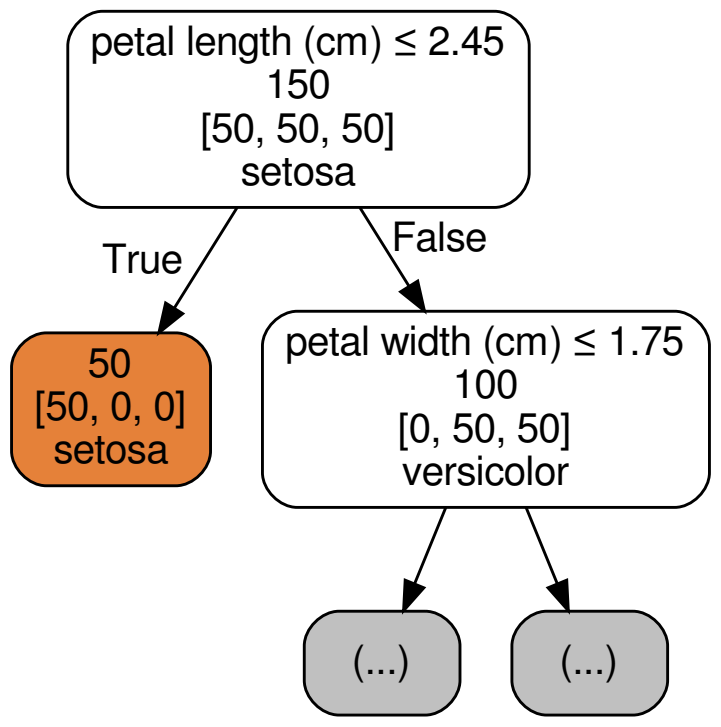
Decision Tree

A method to fit data that generates reasonable decision boundaries

- Relatively fast and easy to fit
- Intuitive to use
- Often over fits data
  - Over fitting may be controlled with pruning
  - Pruning may reduce accuracy
- Large trees are difficult to interpret

Building a Forest of Decision Trees

Make splits in the data in such a way that it separates the classes or that minimizes the distance between the predictions in a region.

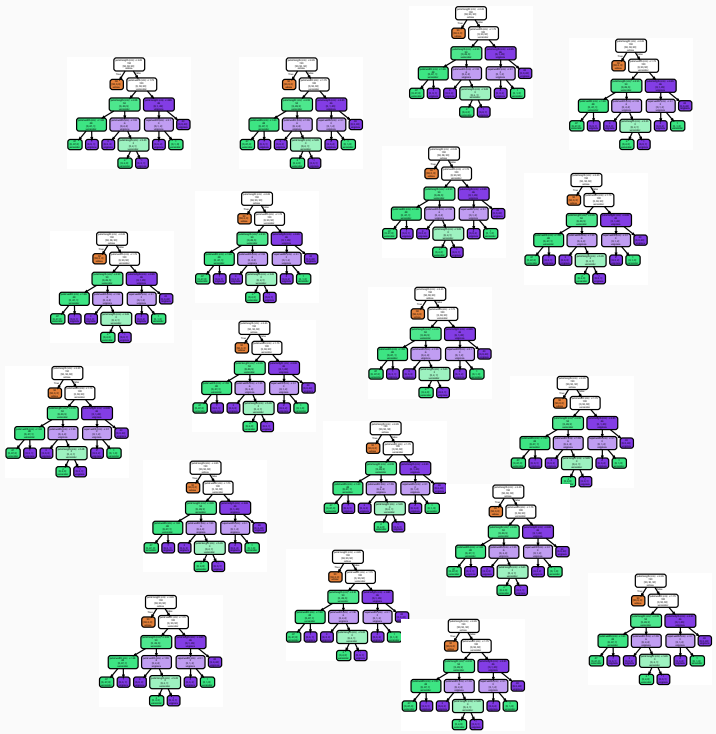


Random Forest

Combine decision trees into an ensemble

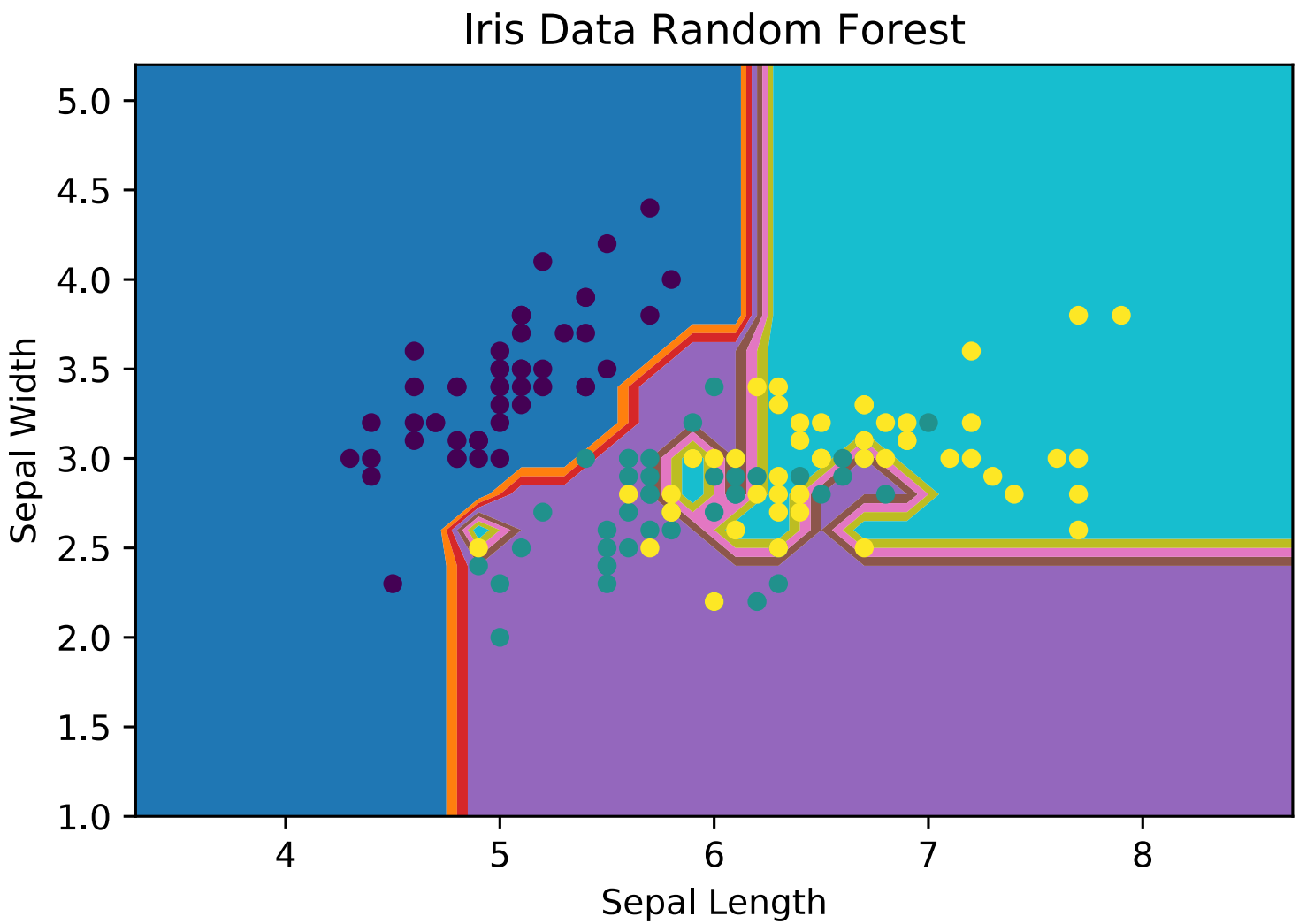
- Work by randomly splitting predictors and data (bagging)
- Make a large number of trees and average their predictions
- Can be optimized with relatively few parameters
- Resulting models can be very large making inference slow
- Models do not fit sparse data well
- Results are difficult to interpret

Figure 7: Decision Tree Example



Random Forest

Random Forest Decision Boundary

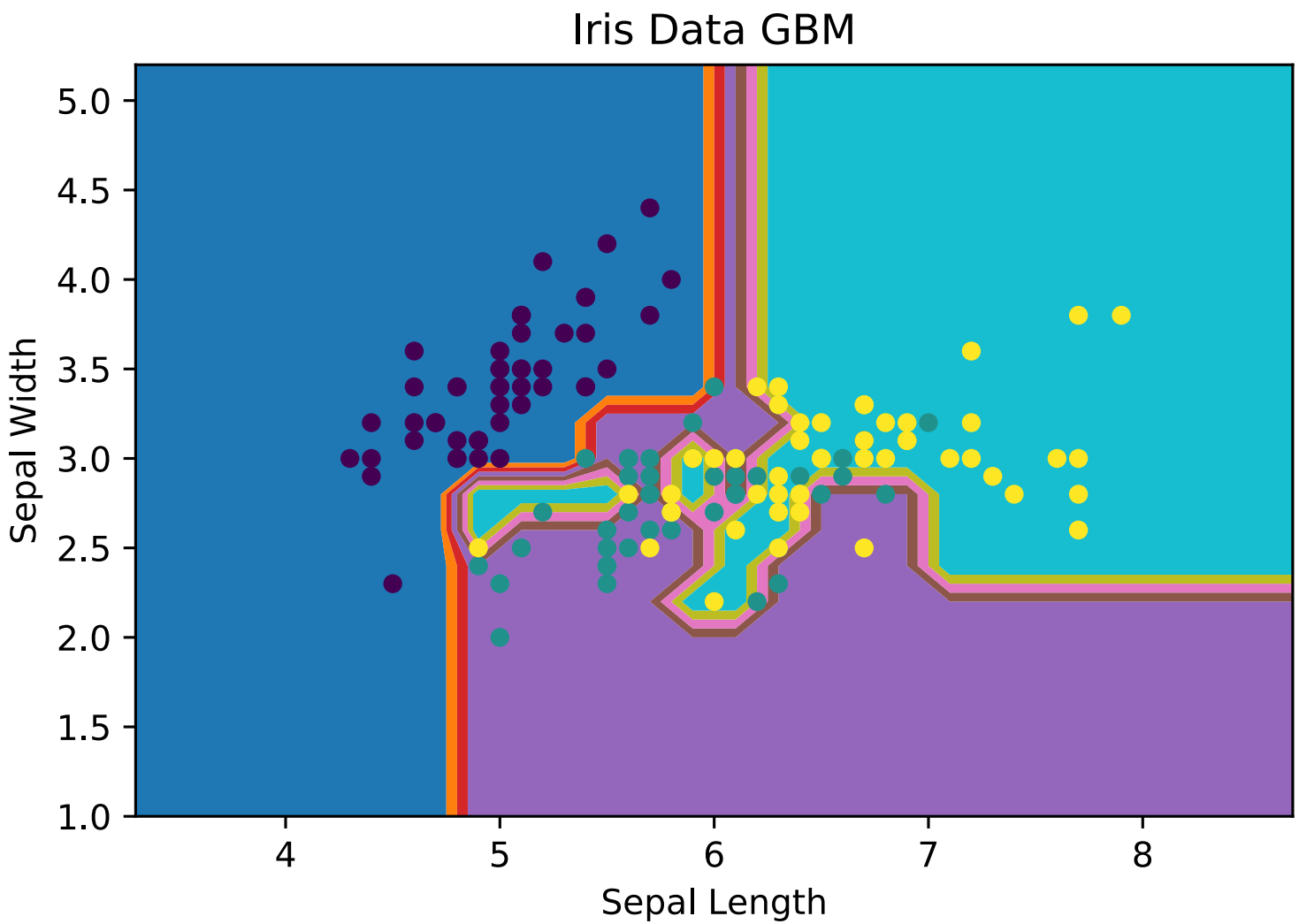


Boosted Trees

Combine short decision trees fitting to the error of the previous tree

- Make an ensemble of weak learners (small decision trees)
- Fit to decision trees to reduce the error of the previous tree
- Models generally have very high accuracy
- Over fitting is common
- Large number of difficult to optimize parameters

GBM Decision Boundary

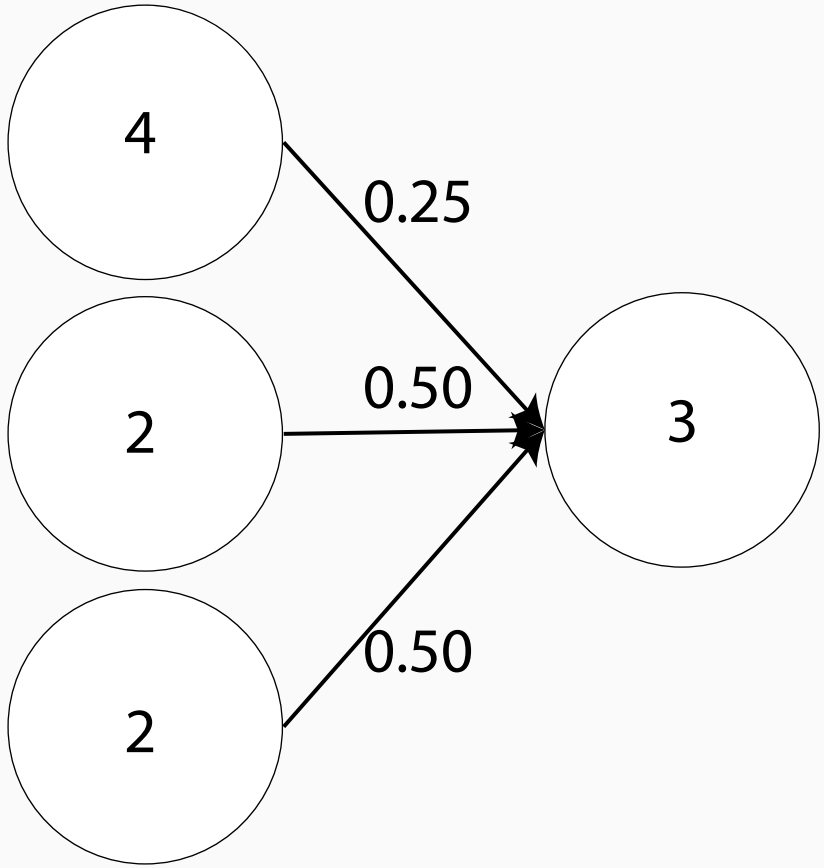


Neural Networks

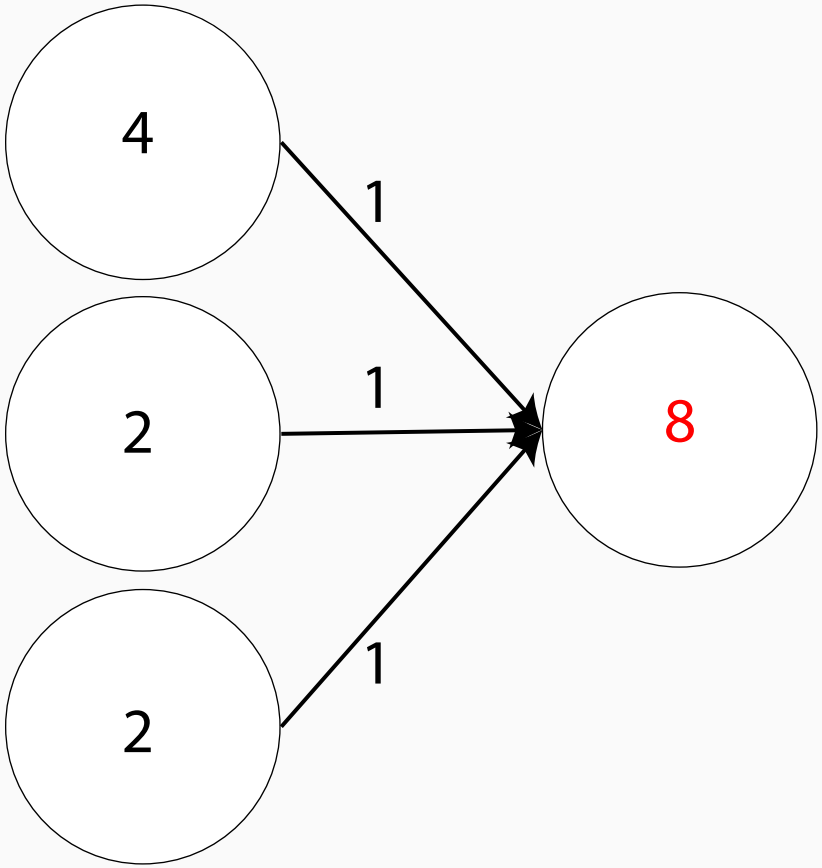
A class of models using collections of linear algebra operations to make predictions, classify data, so called deep learning and perform complex tasks

- Wide-range of applications from classification to self-driving cars
- Automatic variable selection and engineering
- Require extensive fitting
- Computationally intensive
- Many architectures for different applications
- Applications include computer vision, natural language processing, predictions, task learning and speech recognition
- Fundamentally simple operations that when combined solve complex problems

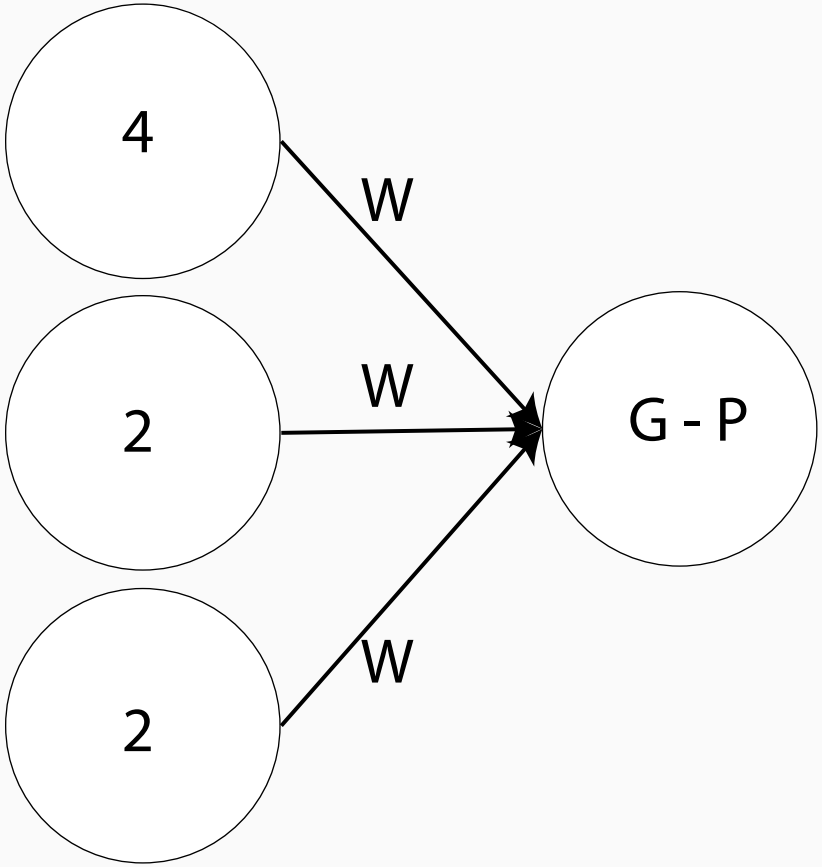
Simplest Neural Network



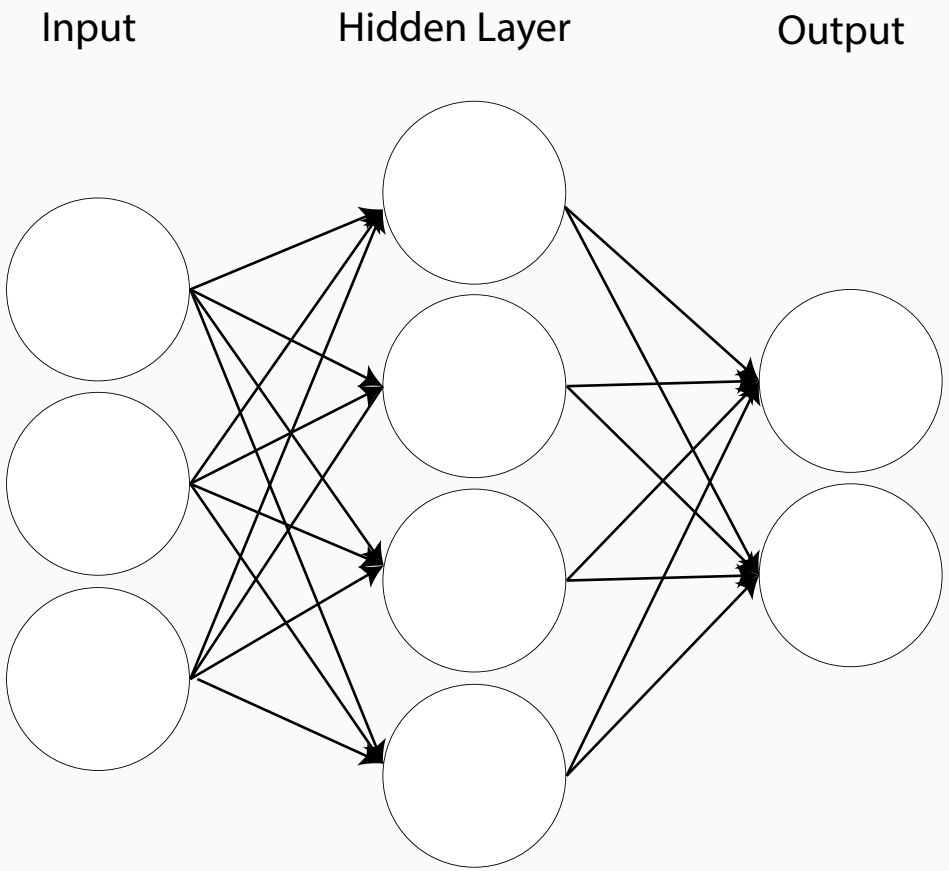
Simplest Neural Network



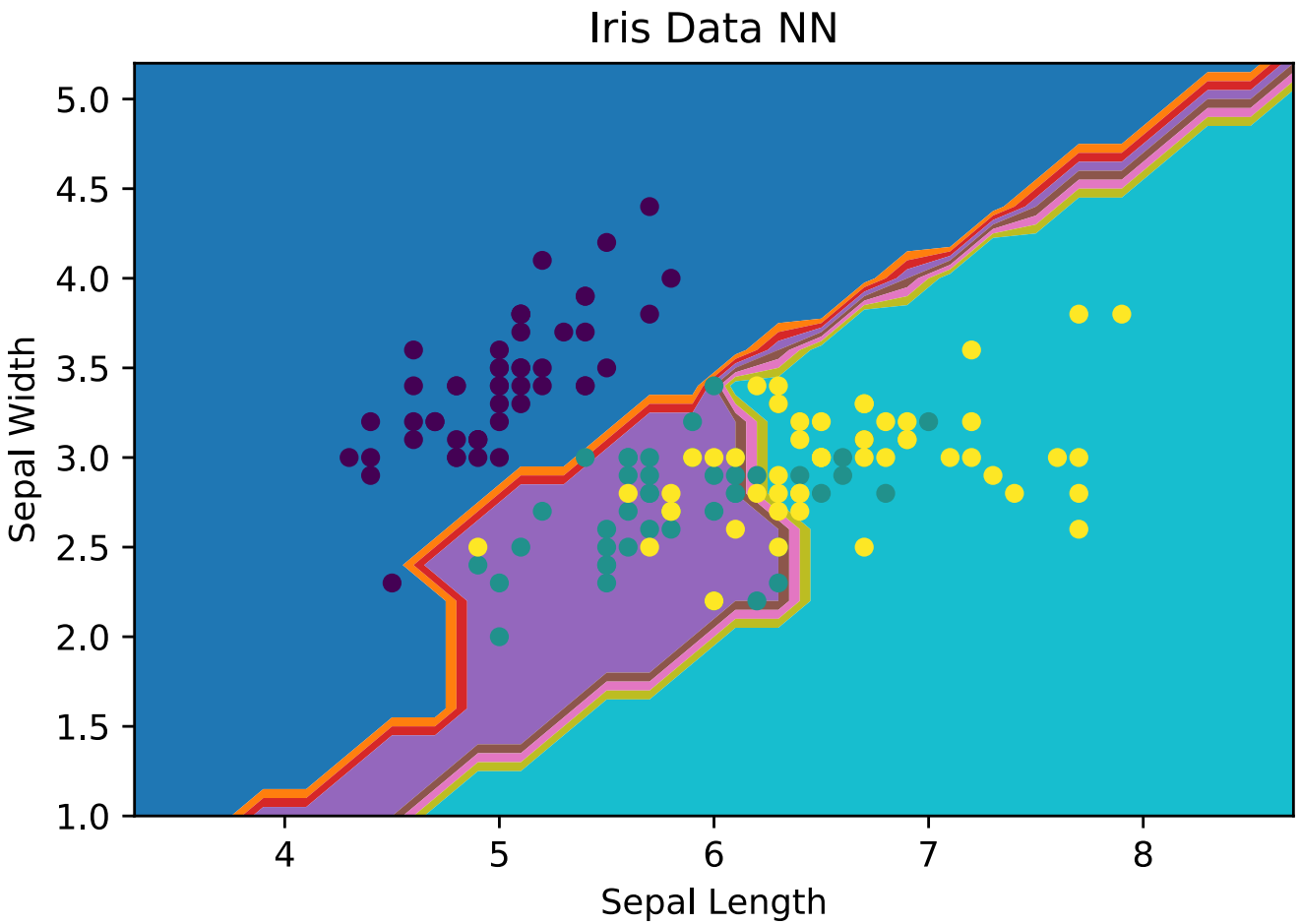
Simplest Neural Network



Simplest Neural Network



Neural Network Decision Boundary



Other Supervised Learning Methods

Many other methods available

- Regularized regression method to control overfitting and reduce variance
- Naive Bayes
- Gaussian Process
- Linear Discriminant Analysis
- k-Nearest Neighbors

Unsupervised Learning

Inferring the structure of unlabeled data

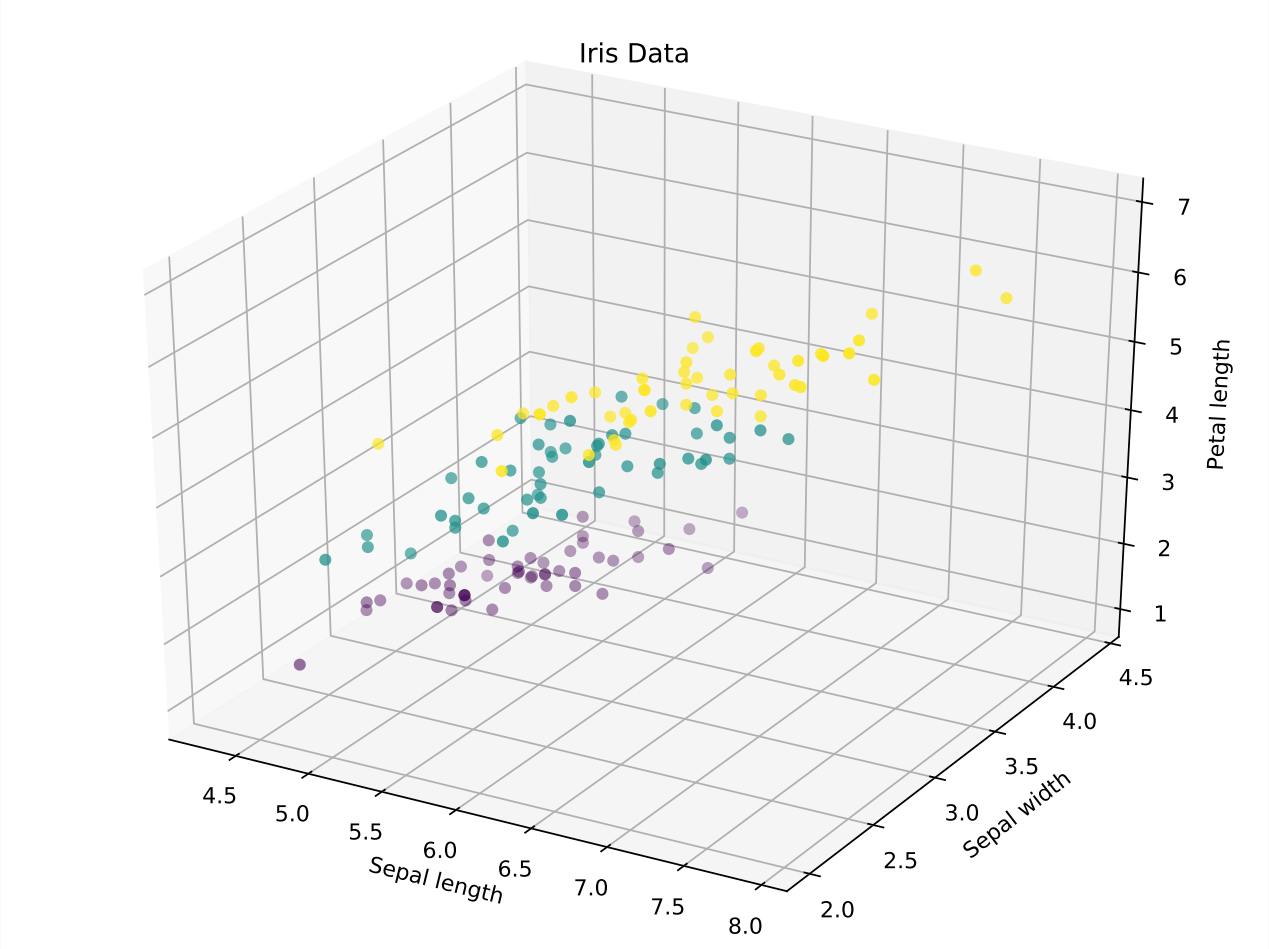
Support Vector Machines and Decision Trees

- Dimensionality Reduction
  - Principle Component Analysis
  - Non-negative Matrix Factorization
  - Latent Dirichlet Allocation
- Clustering
  - K-means
  - Gaussian Mixture Models
  - Manifold Learning

PCA Dimensionality Reduction

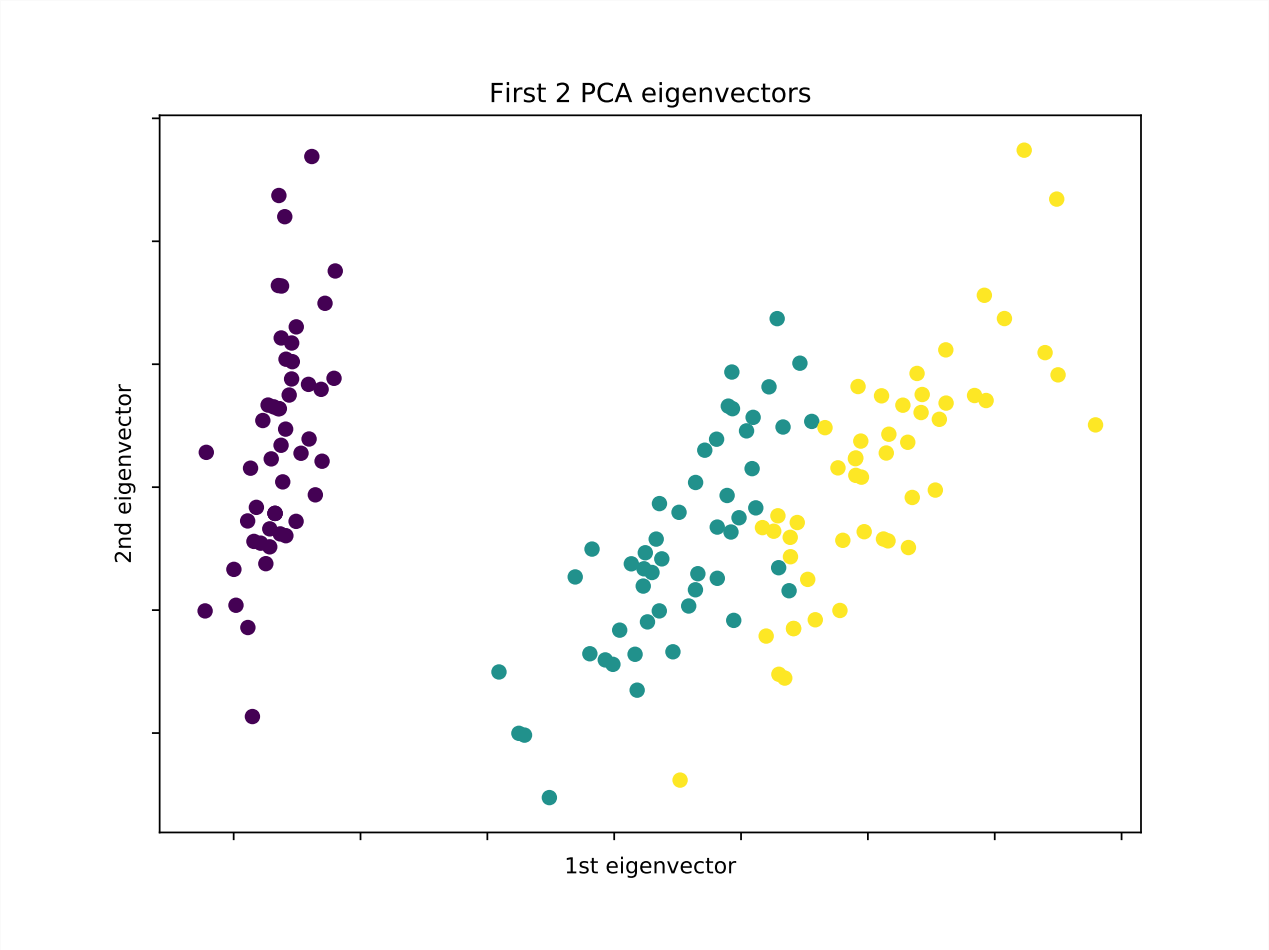
Find the best low dimensional representation of the data

Figure 8: Iris Data with Three Components



PCA

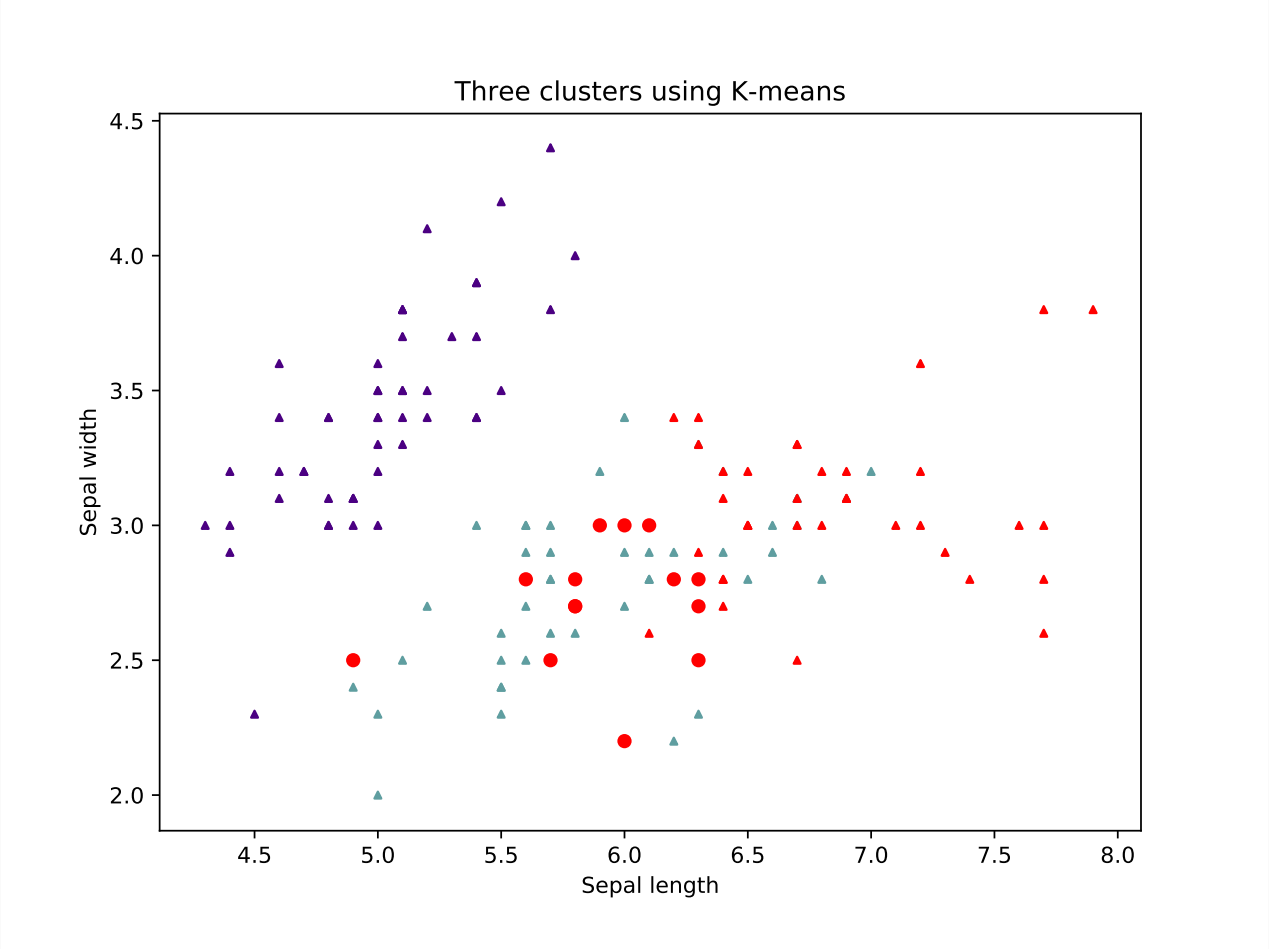
First two PCA eigenvectors



K-means

Find K groupings based on variable similarity.

Figure 9: Iris Data with 3 cluster



Reinforcement Learning

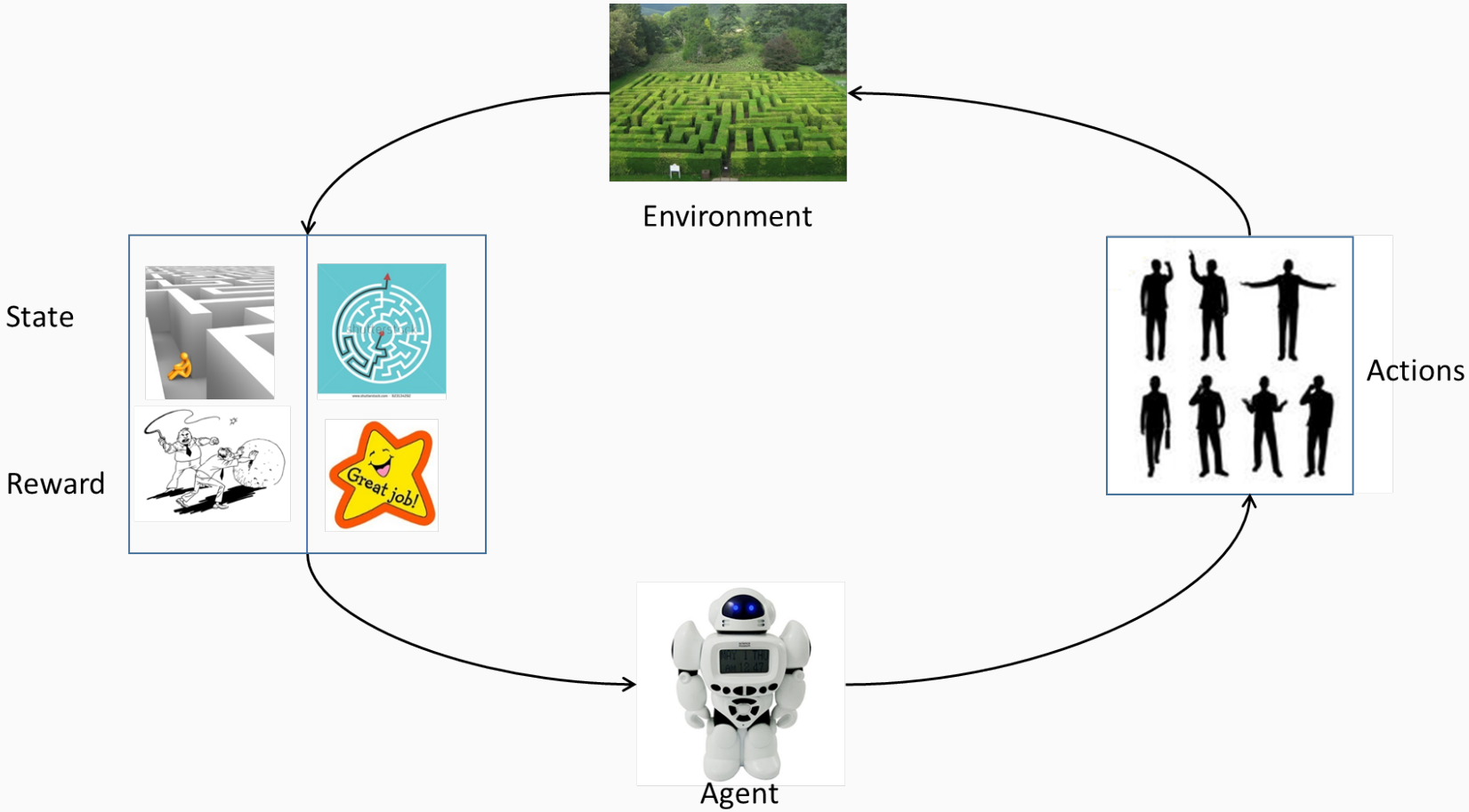
New problem types

What if we know the desired outcome but the data needed to model every possible situation is vast or there the decision is dependent on many changing factors?

- Reinforcement learning is a method to learn a policy to arrive at an outcome rather than learning a labeled value
- Successes include self-driving cars, beating the best in the world at the game of Go and playing most Atari games at superhuman levels
- Must define the actions, the rewards and the states
- Very data intense

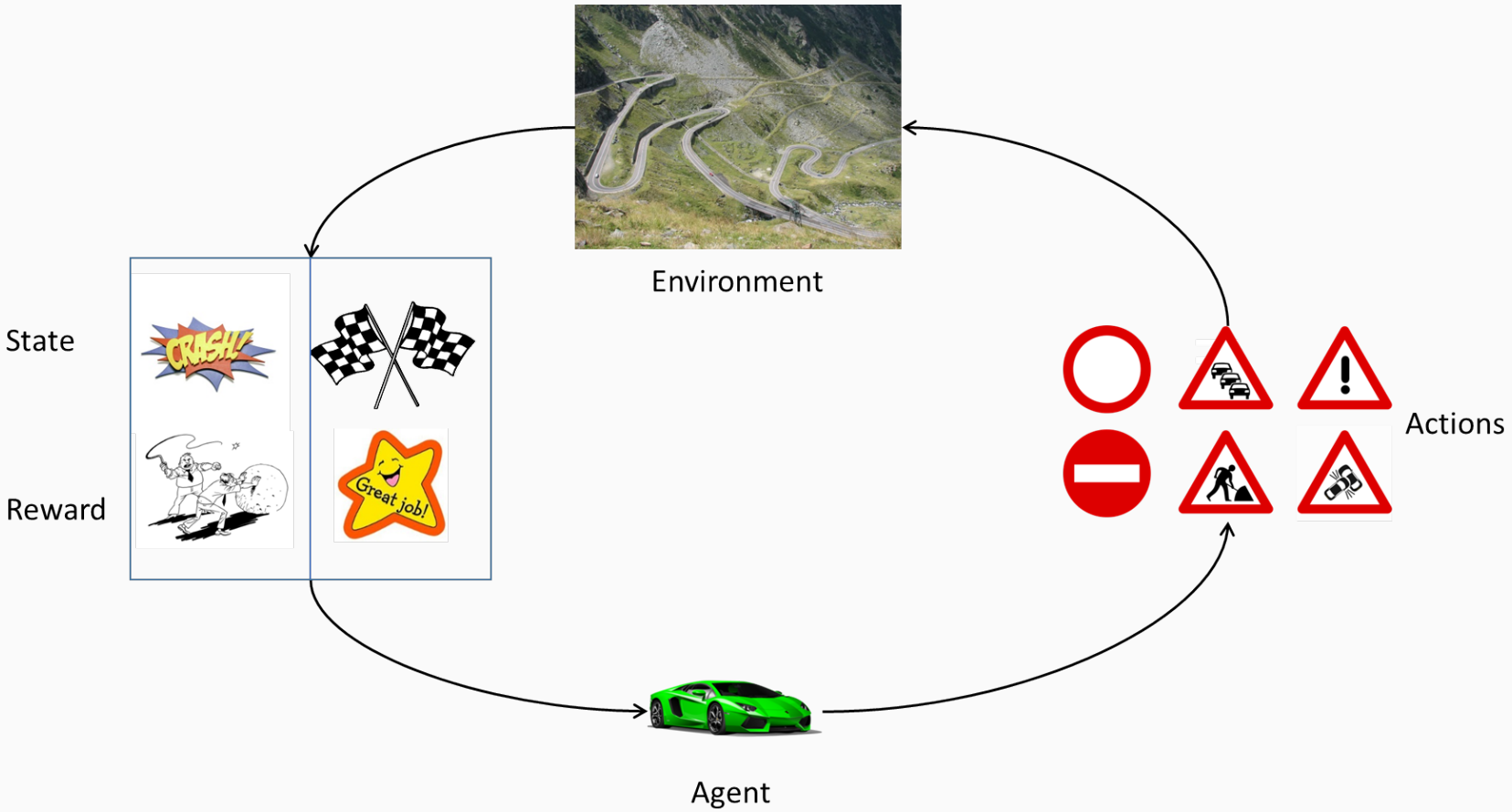
Reinforcement Learning Concept

What if we know the desired outcome but the data needed to model every possible situation is vast or there the decision is dependent on many changing factors?



Reinforcement Learning Example

Self-Driving Race Car

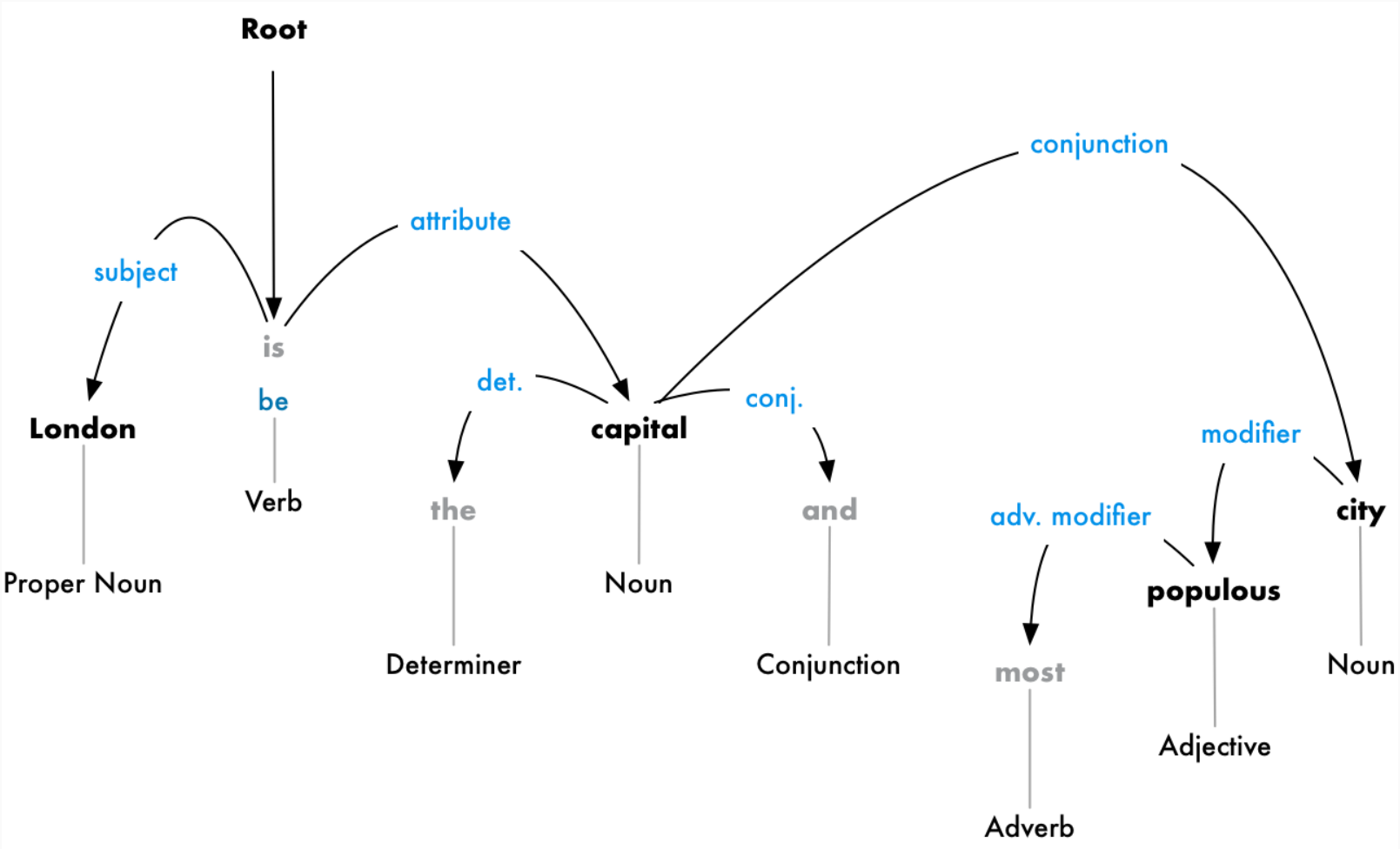


Special Topics

Teaching a computer to read

Computers can't read! Wait can they?

London is the capital and most populous city.



How do computers see?

What about images? What would a machine learning algorithm use to add the labels below?