A Tiny Taste of Machine Learning

Lesson 12

The plan ahead

- Machine learning is a huge topic – with many tertiary modules dedicated to it
  - natural language processing, computational biology, computer vision, robotics, other areas
- In this class, we will
  - provide an introduction to the basic ideas, including ways to measure distances between examples, and how to group examples based on distance to create models
  - introduce classification methods, such as “k nearest neighbor” methods
  - introduce clustering methods, such as “k-means”

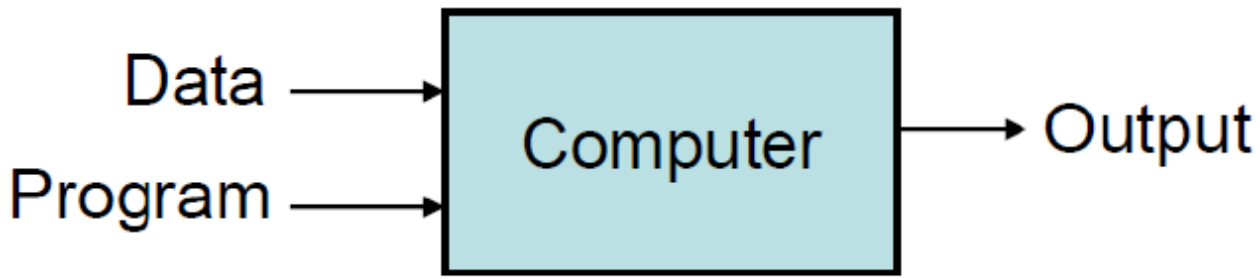
What is Machine Learning

- Many useful programs learn something
- In last few lessons, we used linear regression to learn models of data
- “Field of study that gives computers the ability to learn without being explicitly programmed.” Arthur Samuel
  - Computer pioneer who wrote first self-learning program, which played checkers – learned from “experience”
  - invented alpha-beta pruning – widely used in decision tree searching

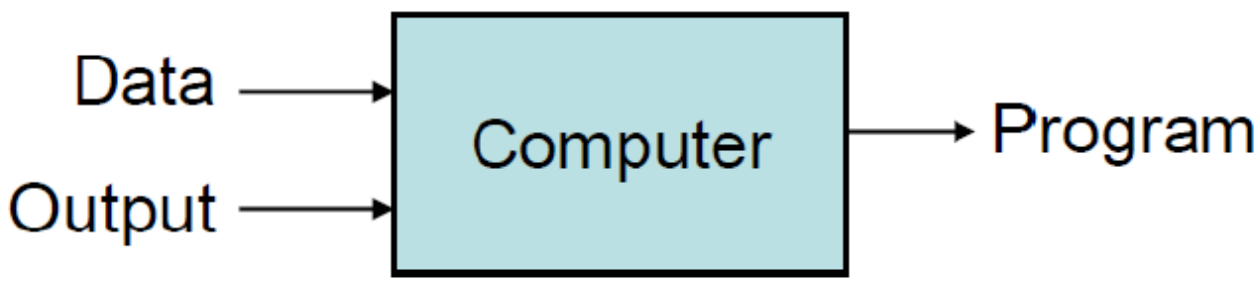
What Is Machine Learning?

- Modern statistics meets optimization

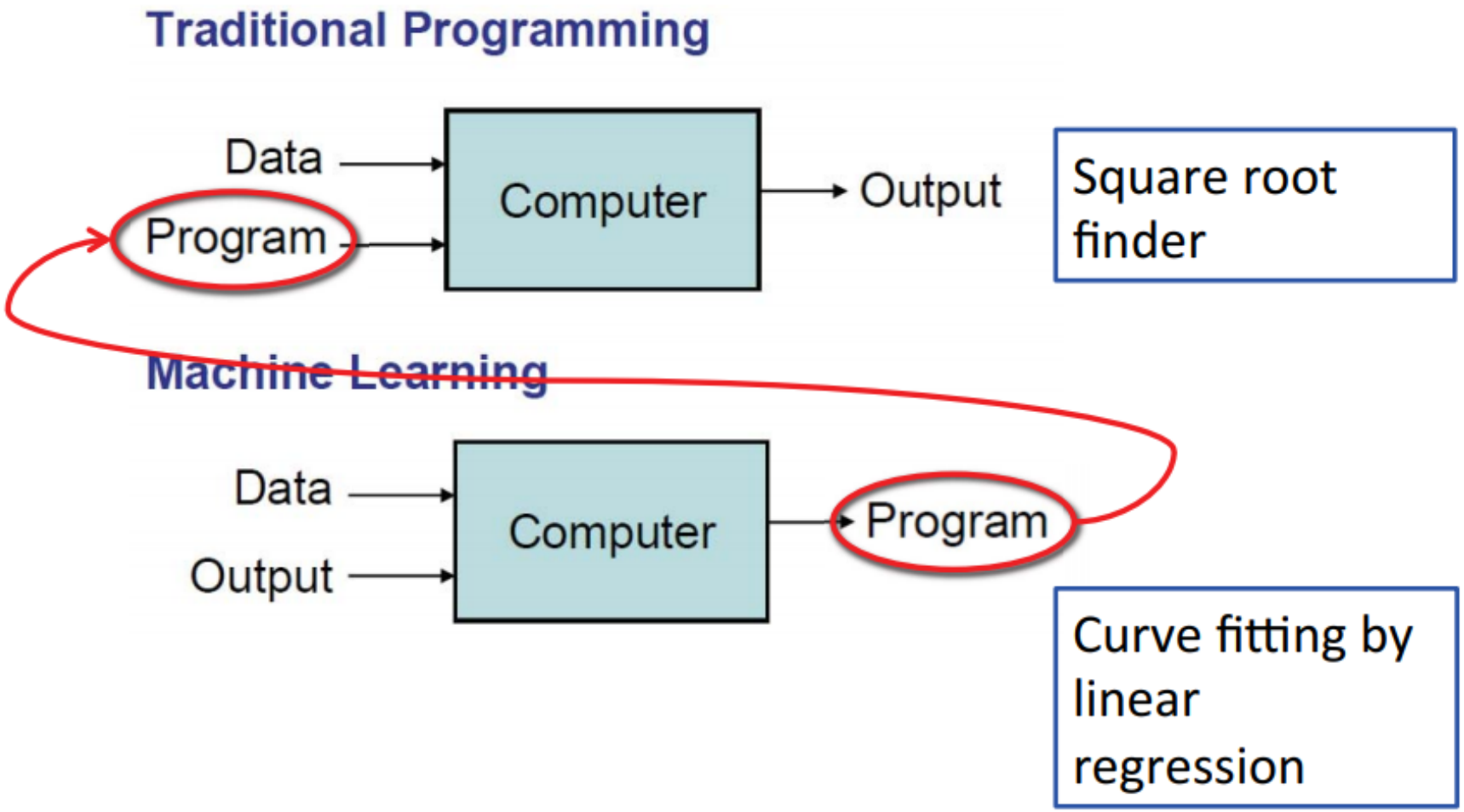
Traditional Programming



Machine Learning



What Is Machine Learning?



How Are Things Learned?

- Memorization
  - Accumulation of individual facts
  - Limited by
    - Time to observe facts
    - Memory to store facts

Declarative knowledge

- Generalization
  - Deduce new facts from old facts
  - Limited by accuracy of deduction process
    - Essentially a predictive activity
    - Assumes that the past predicts the future

Imperative knowledge

- Interested in extending to programs that can infer useful information from **implicit** patterns in data

Basic Paradigm

- Observe set of examples: training data
- Infer something about process that generated that data
- Use inference to make predictions about previously unseen data: test data

Basic Paradigm

- Observe set of examples: training data
- Infer something about process that generated that data
- Use inference to make predictions about previously unseen data: test data

Spatial deviations relative to mass displacements of spring

Fit polynomial curve using linear regression

Predict displacements for other weights

Basic Paradigm

- Observe set of examples: training data
- Infer something about process that generated that data
- Use inference to make predictions about previously unseen data: test data
- Variations on paradigm
  - Supervised: given a set of feature/label pairs, find a rule that predicts the label associated with a previously unseen input
  - Unsupervised: given a set of feature vectors (without labels) group them into "natural clusters" (or create labels for groups)

Football players, labeled by position, with height and weight data

Find canonical model of position, by statistics

Predict position of new players

All ML Methods Require:

- Choosing training data and evaluation method
- representation of the features
- distance metric for feature vectors
- objective function and constraints
- optimization method for learning the model

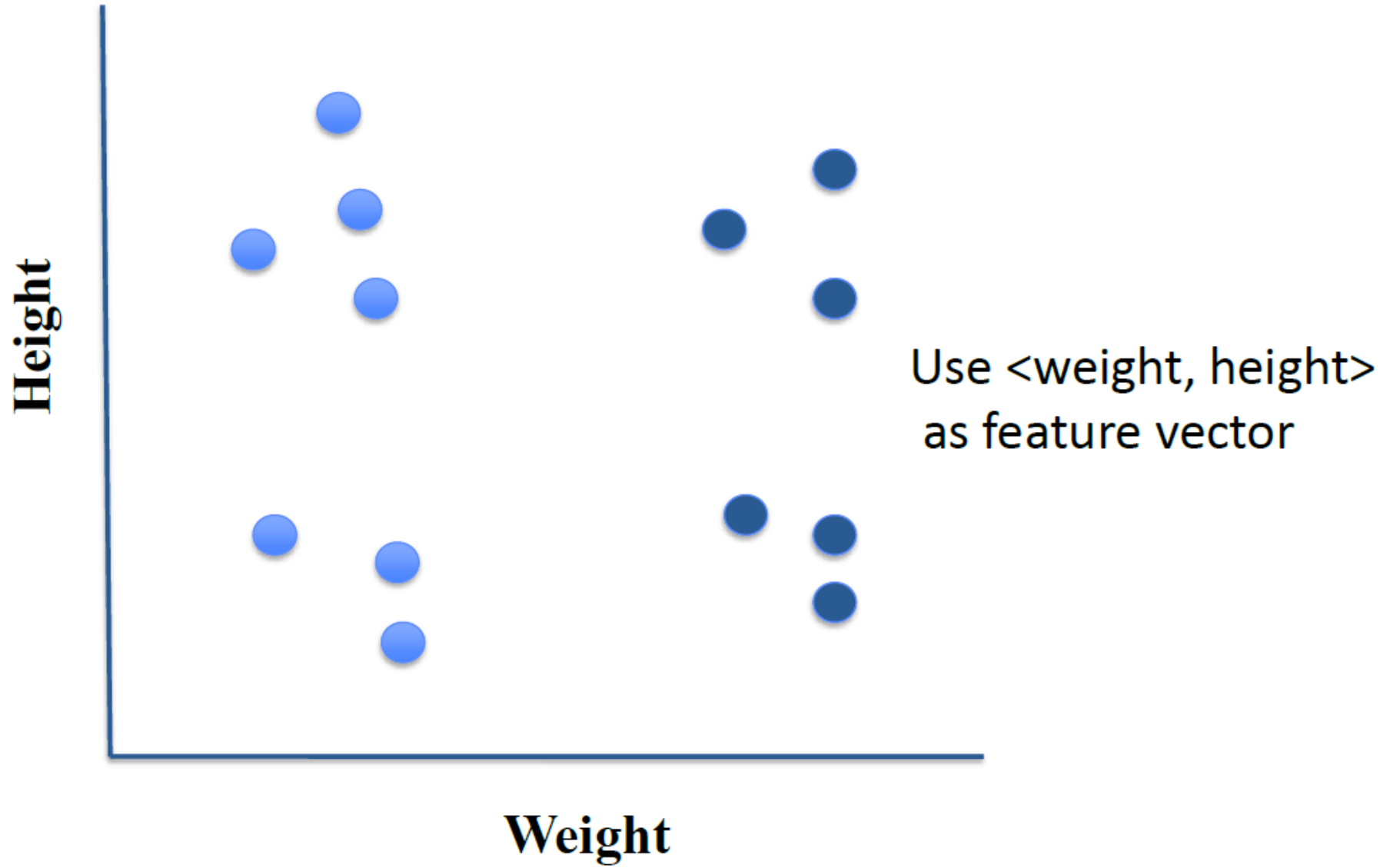
Supervised Learning

- Start with set of feature vector/value pairs
- Goal: find a model that predicts a value for a previously unseen feature vector
- Regression models predict a real
  - As with linear regression
- Classification models predict a label (chosen from a finite set of labels)

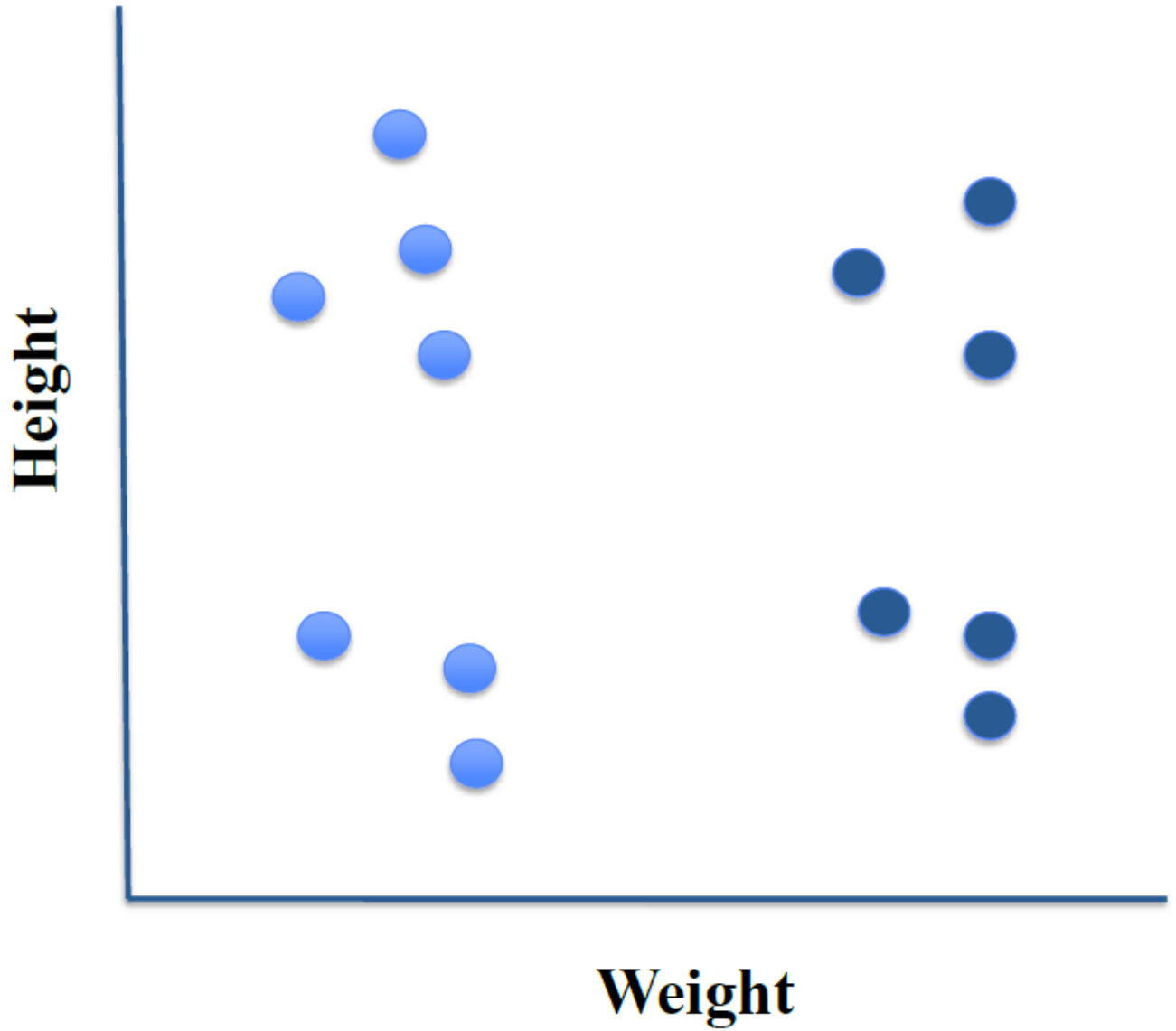
Unsupervised Learning

- Start with a set of feature vectors
- Goal: uncover some latent structure in the set of feature vectors
- Clustering the most common technique
  - Define some metric that captures how similar one feature vector is to another
  - Group examples based on this metric

Some Unlabeled 2D Data

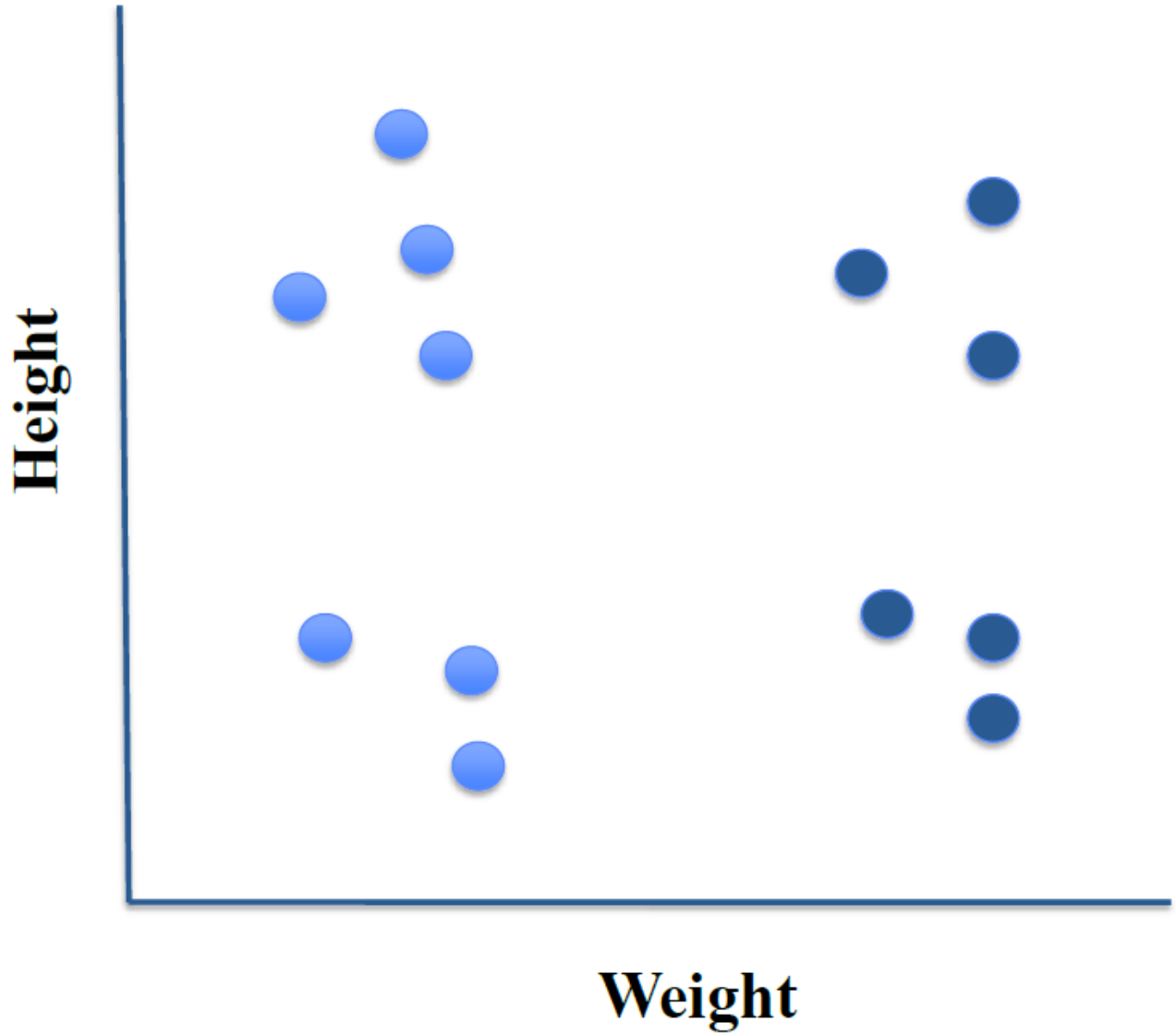


Some Unlabeled 2D Data



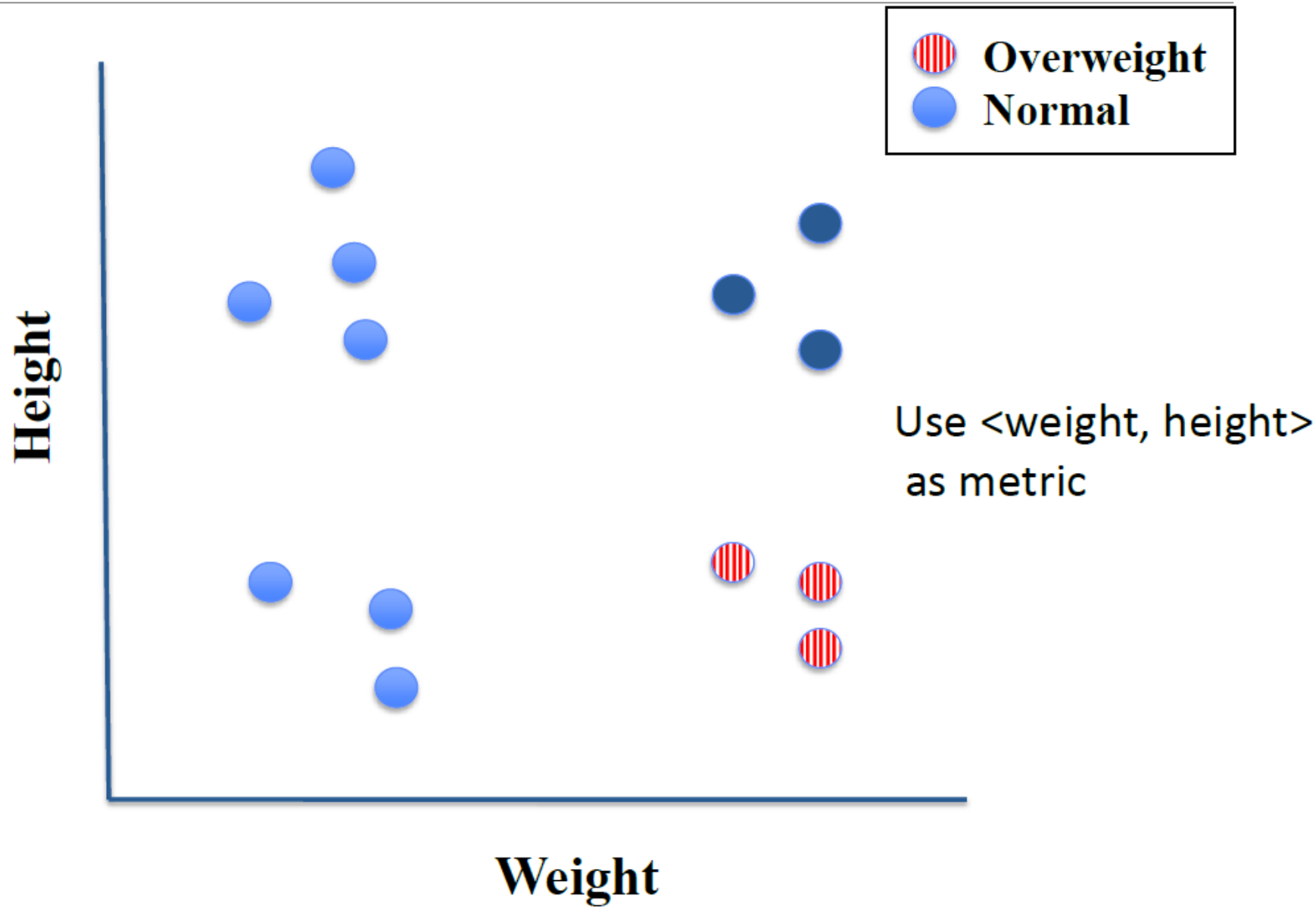
Use weight as feature vector

Some Unlabeled 2D Data



Use height as feature

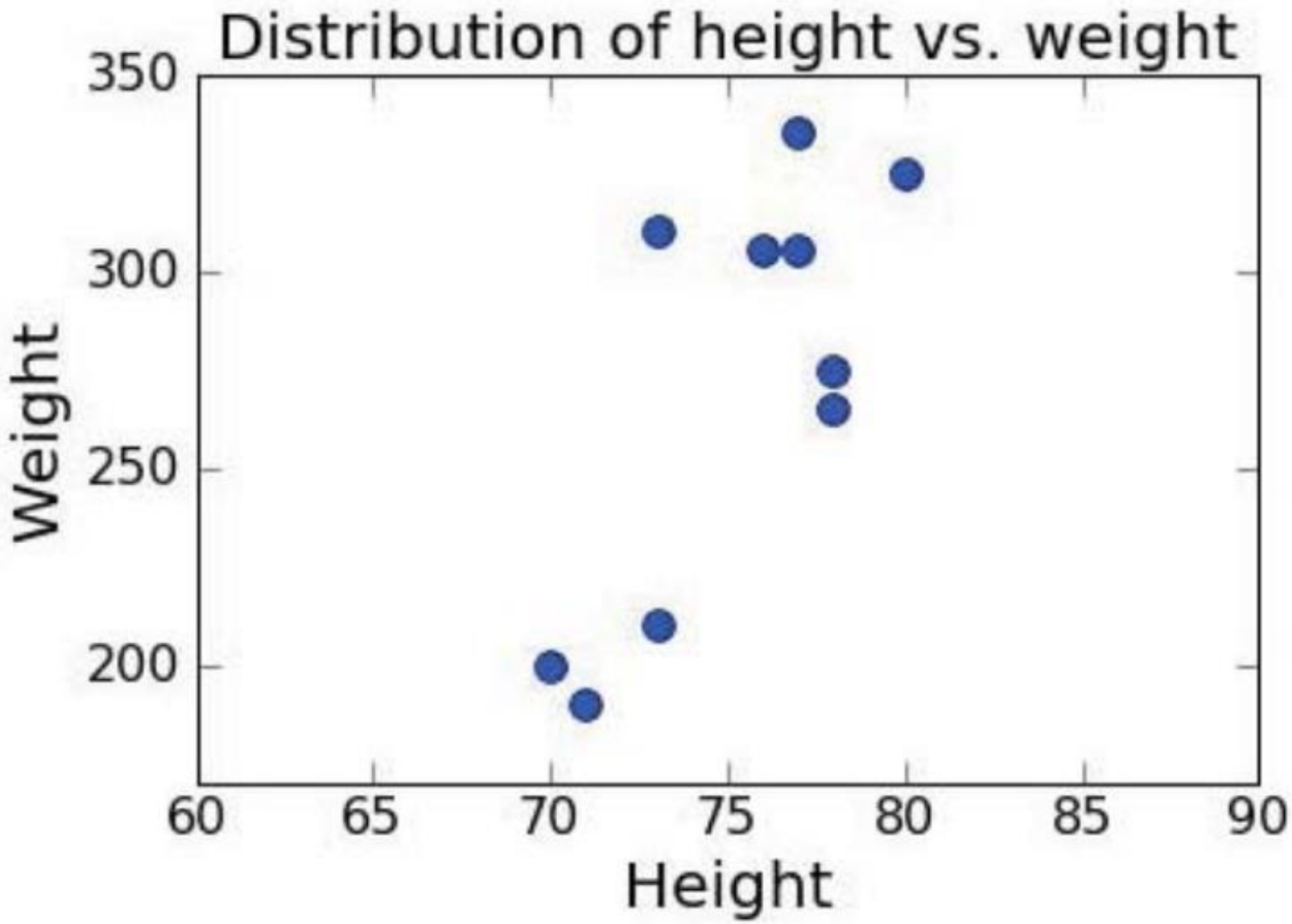
Suppose Data Is Labeled



Some Examples of Classifying and Clustering

- Here are some data on some Athletes from Track and Fields
  - Name, Height, Weight
  - Labeled by type of Events
- Sprinters
  - Edelman = [‘Edelman’,70,200]
  - Hogan = [‘Hogan’,73,210]
  - gronkowski = [‘gronkowski’,78,265]
  - amendola = [‘amednola’,71,190]
  - bennett = [‘bennett’,78,275]
- Javelin Thrower
  - cannon = [‘cannon’,77,335]
  - solder = [‘solder’,80,325]
  - mason = [‘mason’,73,310]
  - thuney = [‘thuney’,77,305]
  - karras = [‘karras’,76,305]

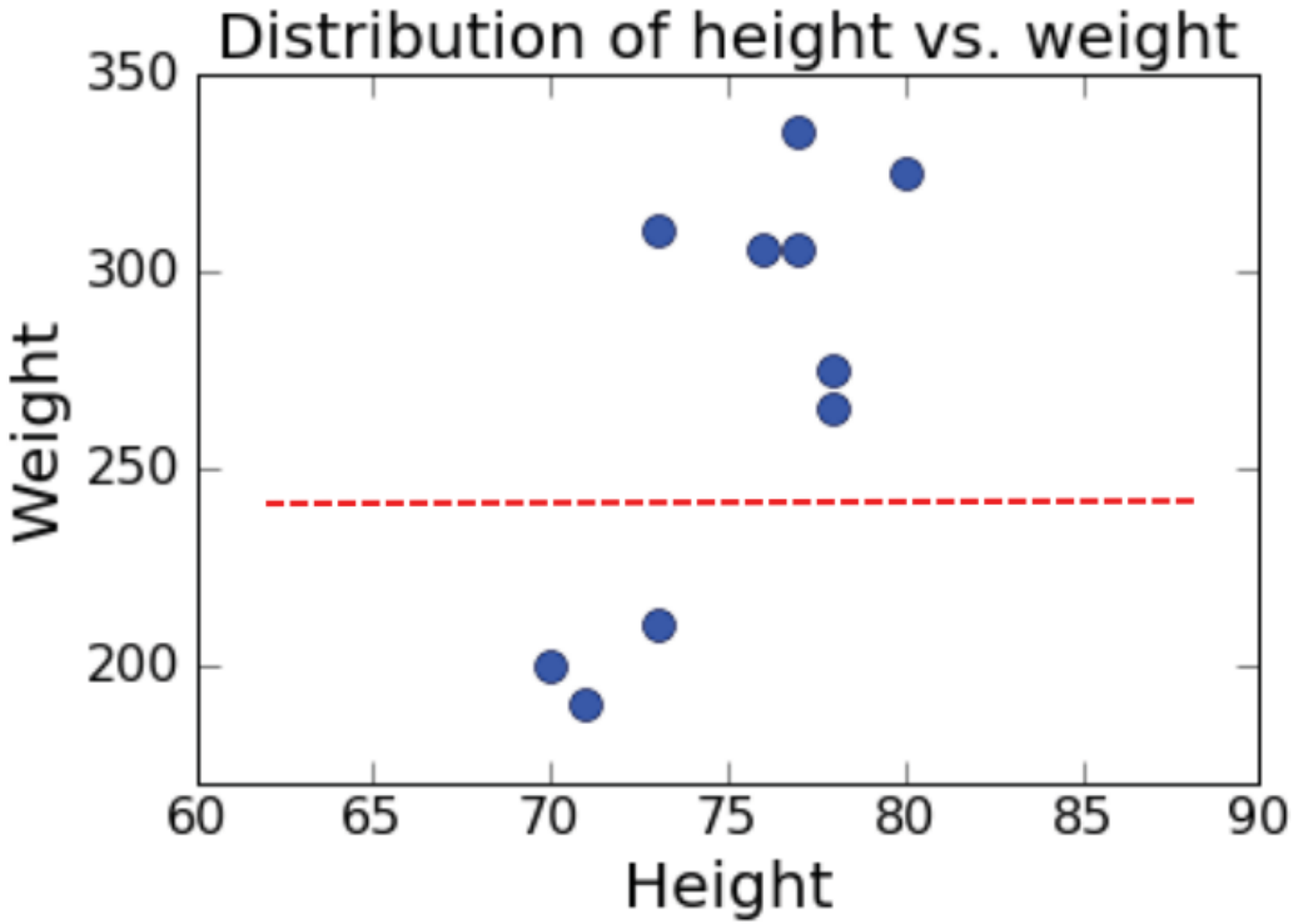
Unlabeled Data



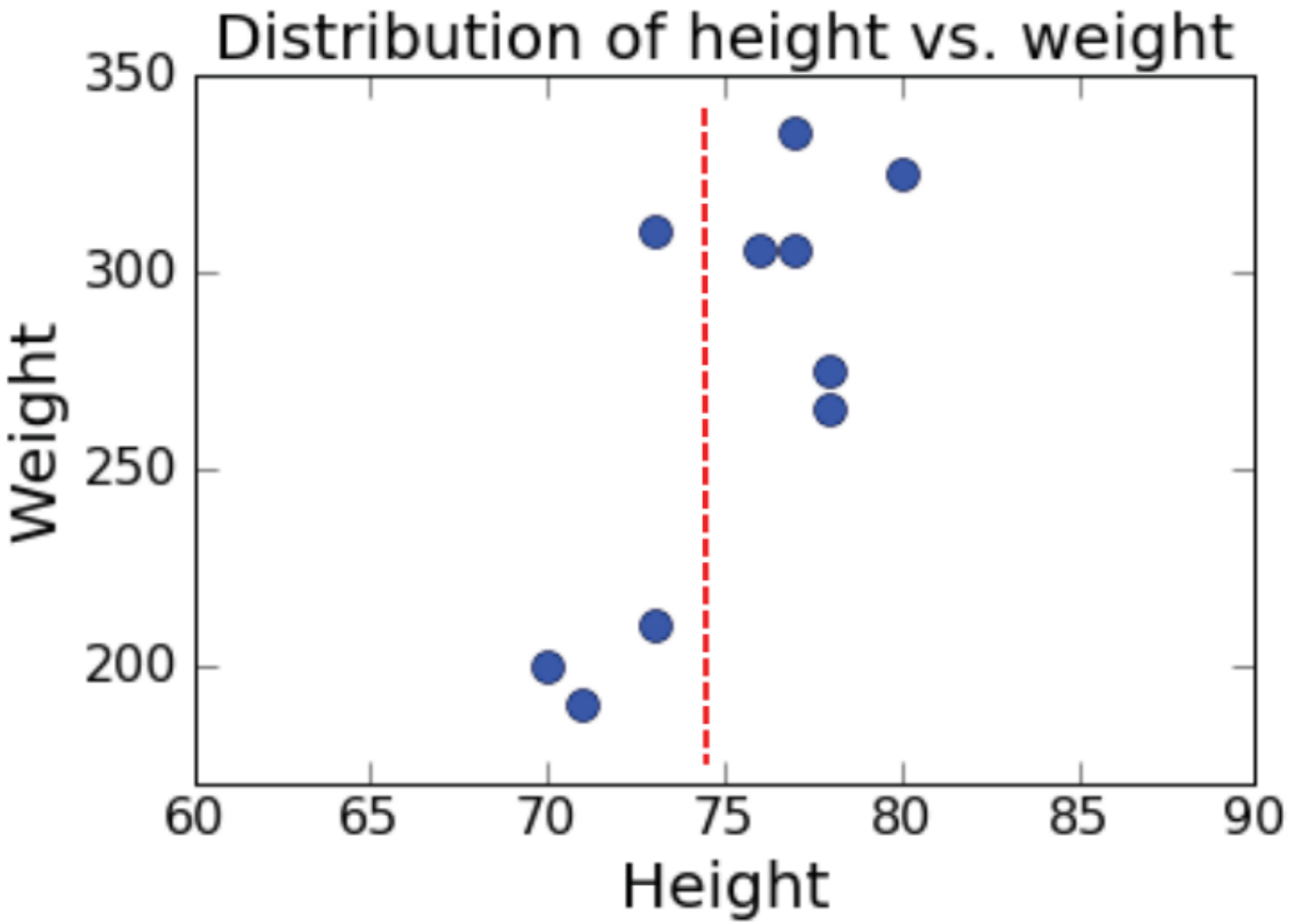
Clustering examples into groups

- Want to decide on "similarity" of examples, with goal of separating into distinct, "natural", groups
  - Similarity is a distance measure
- Suppose we know that there are k different groups in our training data, but don't know labels (here k = 2)
  - Pick k samples (at random?) as exemplars
  - Cluster remaining samples by minimizing distance between samples in same cluster (objective function) – put sample in group with closest exemplar
  - Find median example in each cluster as new exemplar
  - Repeat until no change

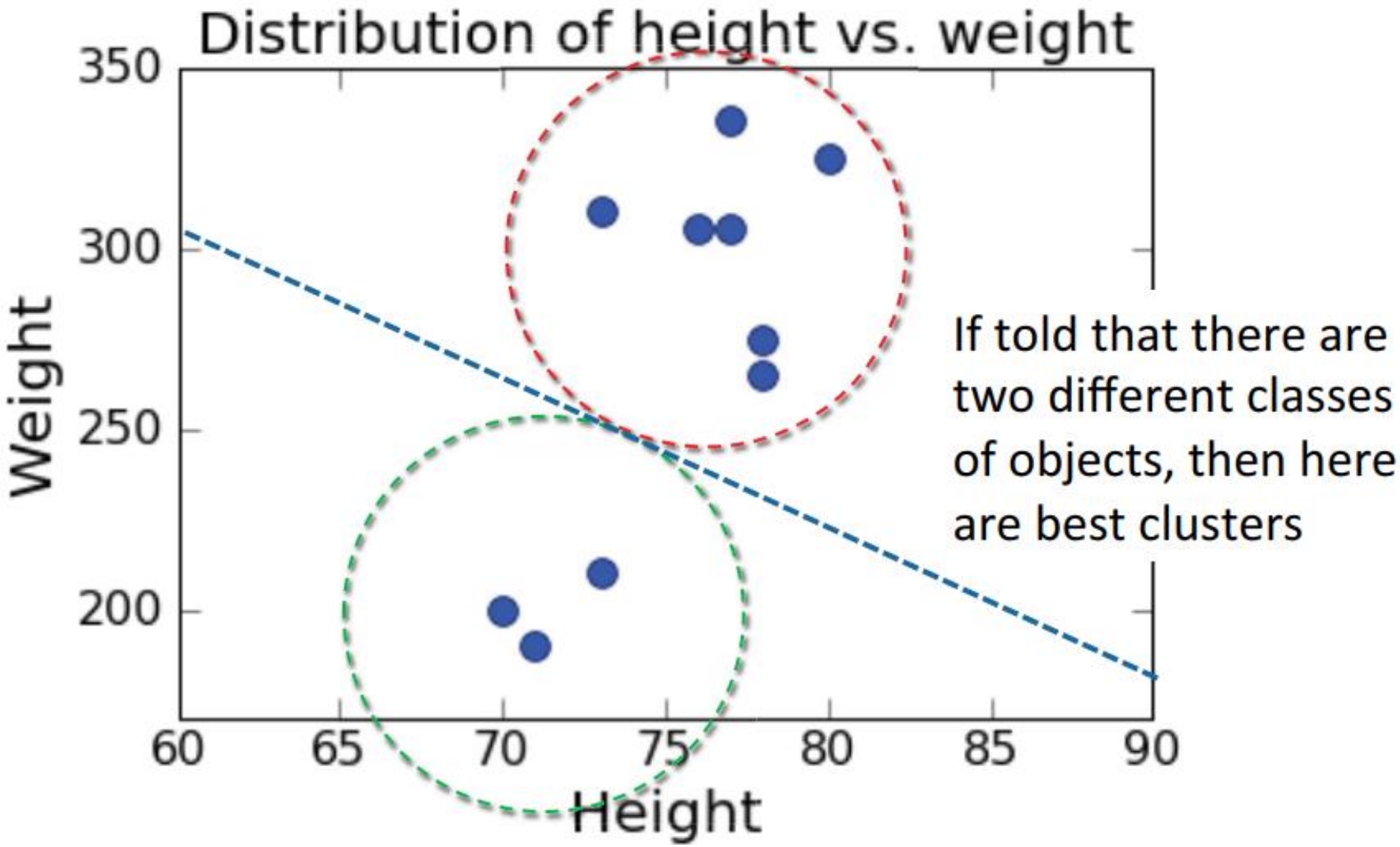
Similarity Based on Weight



Similarity Based on Height

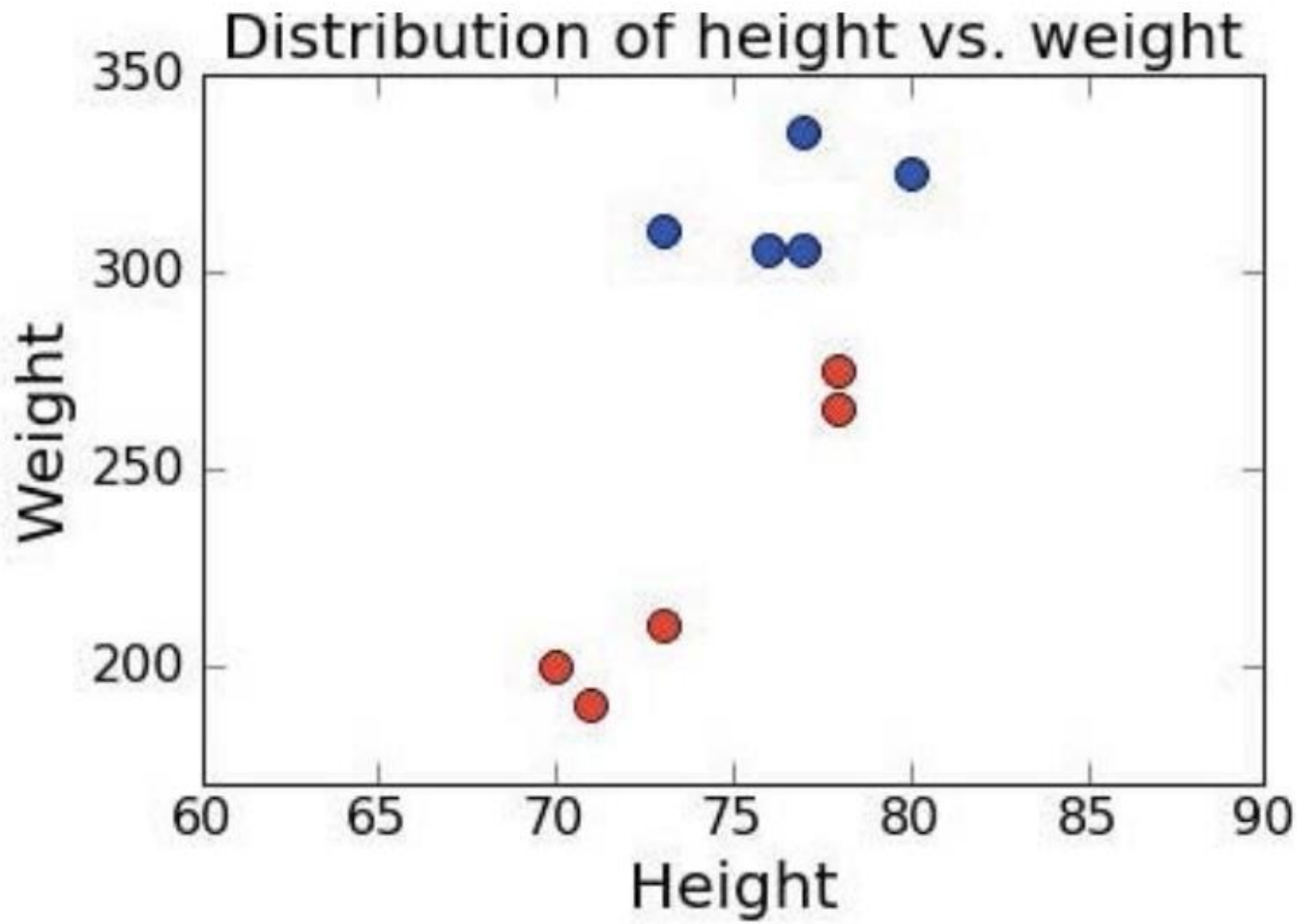


Cluster into Two Groups Using Both Attributes



If told that there are two different classes of objects, then here are best clusters

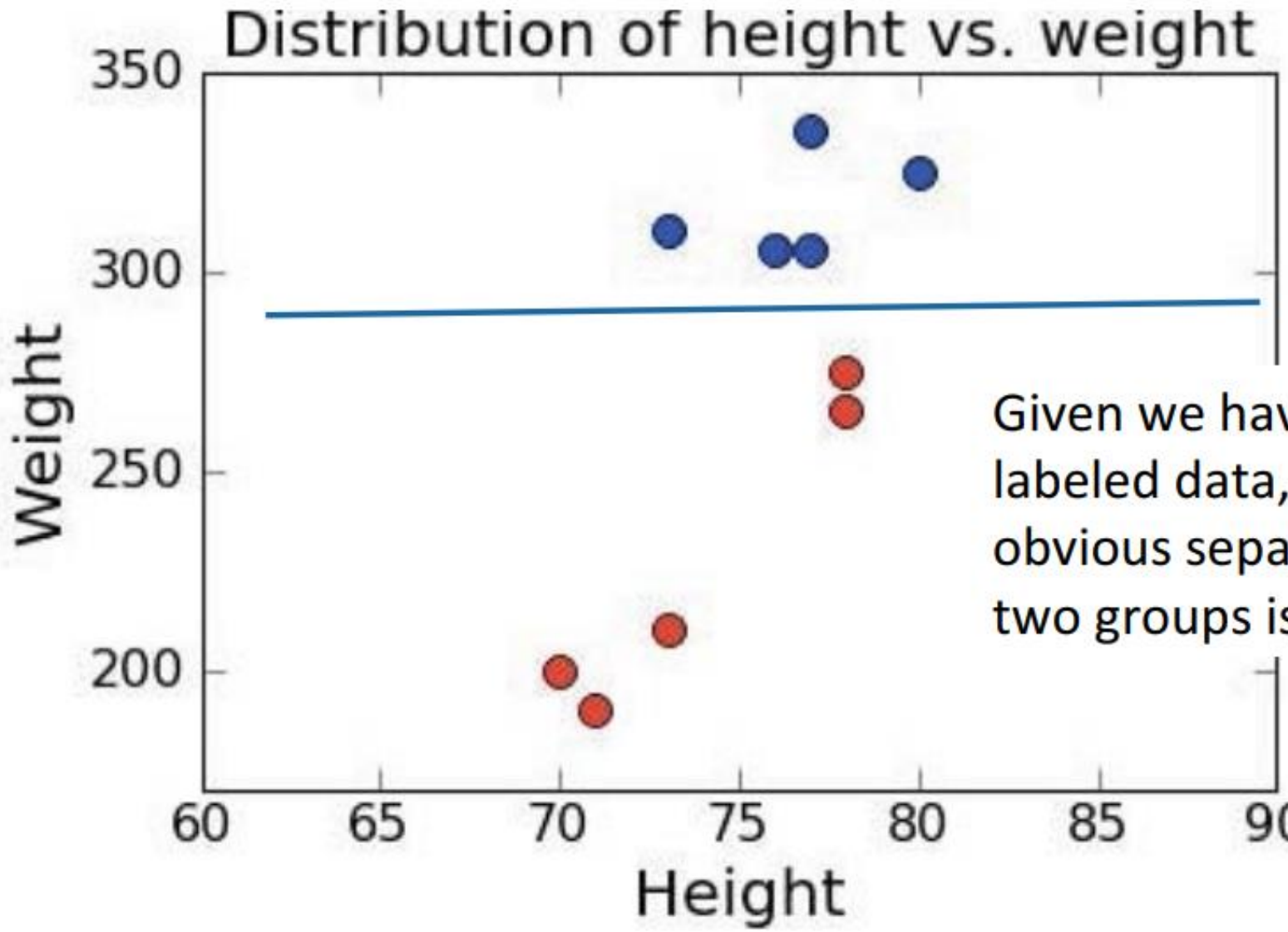
Suppose Data Was Labeled



Finding Classifier Surfaces

- Given labeled groups in feature space, want to find subsurface in that space that separates the groups
  - Subject to constraints on complexity of subsurface
- In this example, have 2D space, so find line (or connected set of line segments) that best separates the two groups
- When examples well separated, this is straightforward
- When examples in labeled groups overlap, may have to trade off false positives and false negatives

Suppose Data Was Labeled

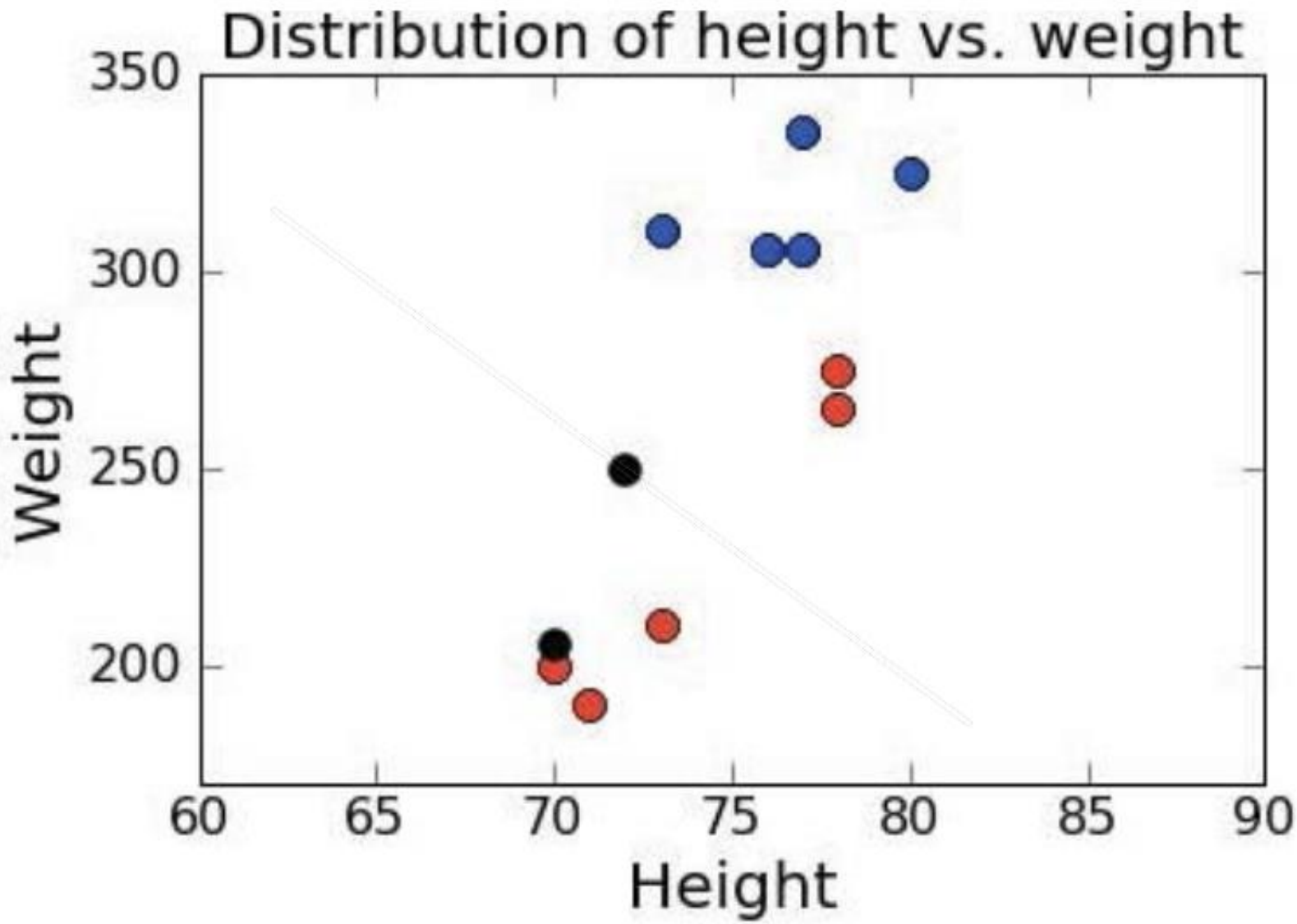


Given we have labeled data, then an obvious separator of two groups is shown

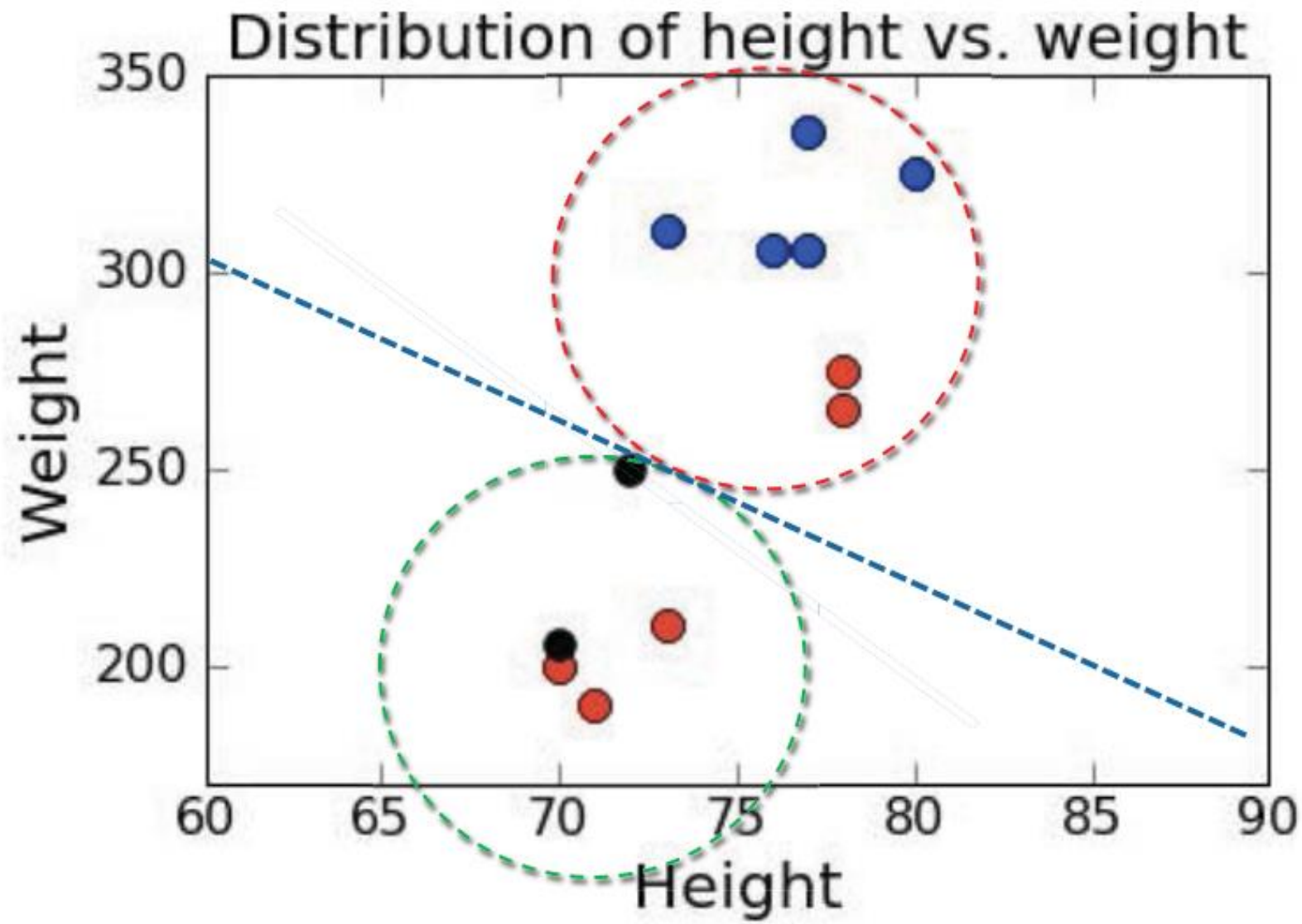
Adding Some New Data

- Suppose we have learned to separate Sprinters and Javelin Throwers
- Now we are given some long jumpers, and want to use model to decide if they are more like Sprinters or Javelin Throwers
  - blount = [‘blount’,72,250]
  - white = [‘white’,70,205]

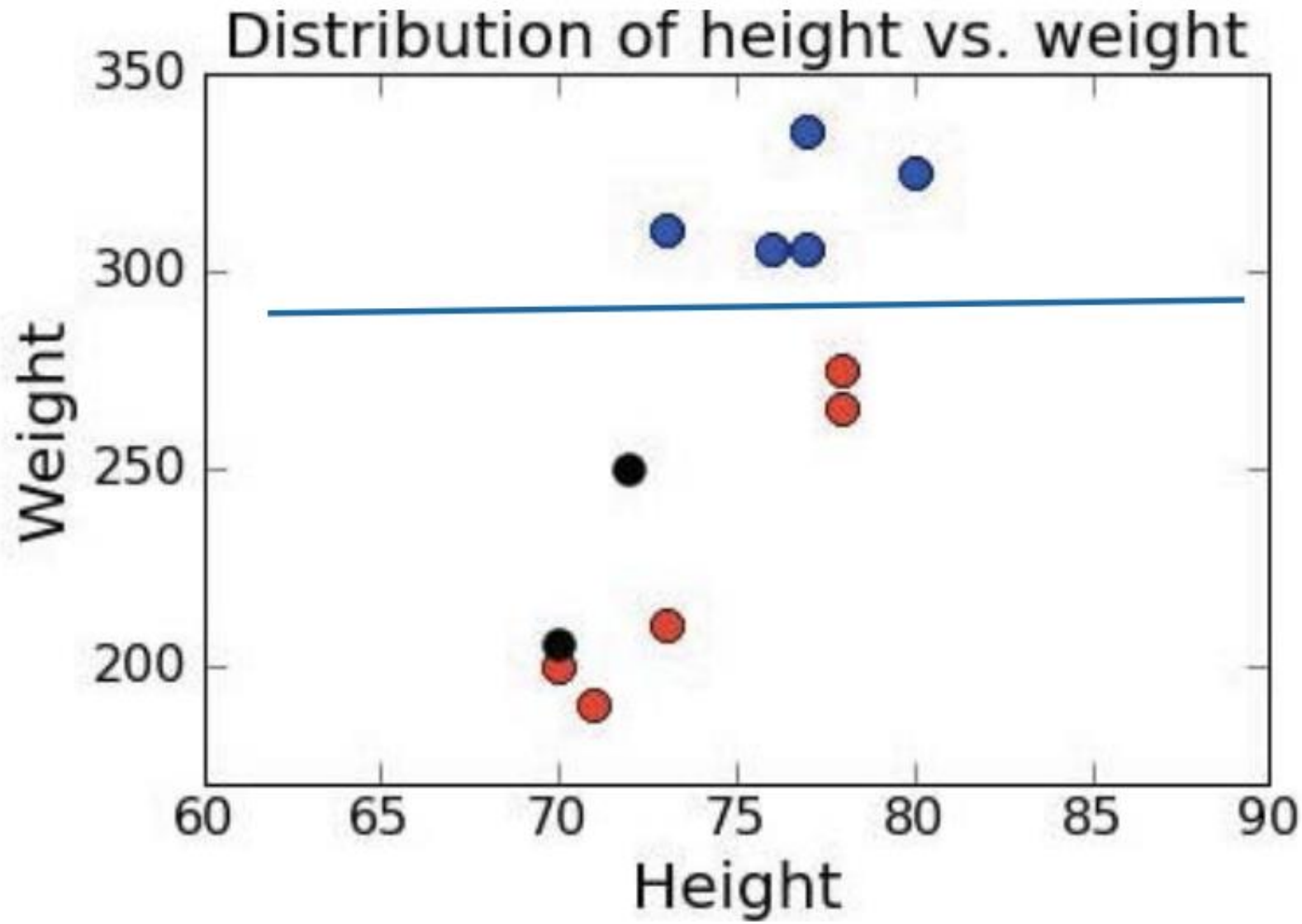
Adding Some New Data



Clustering using Unlabeled Data



Classified using Labeled Data



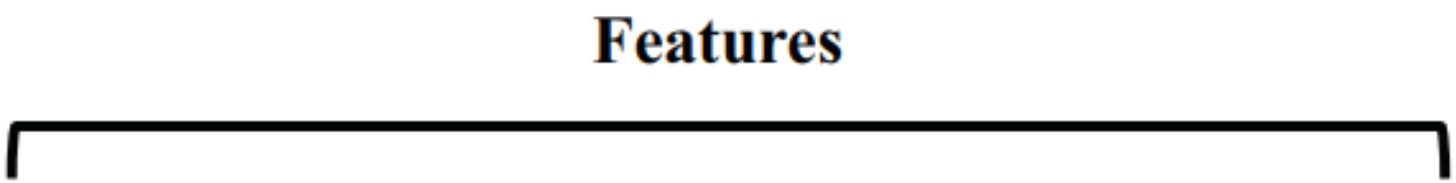
Machine Learning Methods

- We will see some examples of machine learning methods:
- Learn models based on unlabeled data, by clustering training data into groups of nearby points
  - Resulting clusters can assign labels to new data
- Learn models that separate labeled groups of similar data from other groups
  - May not be possible to perfectly separate groups, without “over fitting”
  - But can make decisions with respect to trading off “false positives” versus “false negatives”
  - Resulting classifiers can assign labels to new data

Choosing Features

- Features never fully describe the situation
  - “All models are wrong, but some are useful.” – George Box
- Feature engineering
  - Represent examples by feature vectors that will facilitate generalization
  - Suppose I want to use 100 examples from past to predict at the start of the year, which students will pass the final exam
  - Some features surely helpful, e.g., their grade on the mid year exam, did they do problem sets, etc.
  - others might cause me to overfit, e.g., birth month, eye colour
- want to maximize ratio of useful input to irrelevant input
  - Signal-to-Noise Ratio (SNR)

An Example



Name	Egg-laying	Scales	Poisonous	Cold-blooded	# legs	Reptile
Cobra	True	True	True	True	0	Yes

Initial model:

- Not enough information to generalize

An Example

Features **Label**

Name	Egg-laying	Scales	Poisonous	Cold-blooded	# legs	Reptile
Cobra	True	True	True	True	0	Yes
Rattlesnake	True	True	True	True	0	Yes

Initial model:

- Egg laying
- Has scales
- Is poisonous
- Cold blooded
- No legs

An Example

	Features					Label
Name	Egg-laying	Scales	Poisonous	Cold-blooded	# legs	Reptile
Cobra	True	True	True	True	0	Yes
Rattlesnake	True	True	True	True	0	Yes
Boa constrictor	False	True	False	True	0	Yes

Current model:

- Has scales
- Cold blooded
- No legs

Boa doesn't fit model, but is labeled as reptile.
Need to refine model

An Example

	Features					Label
Name	Egg-laying	Scales	Poisonous	Cold-blooded	# legs	Reptile
Cobra	True	True	True	True	0	Yes
Rattlesnake	True	True	True	True	0	Yes
Boa constrictor	False	True	False	True	0	Yes
Chicken	True	True	False	False	2	No

Current model:

- Has scales
- Cold blooded
- No legs

An Example

	Features					Label
Name	Egg-laying	Scales	Poisonous	Cold-blooded	# legs	Reptile
Cobra	True	True	True	True	0	Yes
Rattlesnake	True	True	True	True	0	Yes
Boa constrictor	False	True	False	True	0	Yes
Chicken	True	True	False	False	2	No
Alligator	True	True	False	True	4	Yes

Current model:

- Has scales
- Cold blooded
- Has 0 or 4 legs

Alligator doesn't fit model, but is labeled as reptile.
Need to refine model

An Example

	Features					Label
Name	Egg-laying	Scales	Poisonous	Cold-blooded	# legs	Reptile
Cobra	True	True	True	True	0	Yes
Rattlesnake	True	True	True	True	0	Yes
Boa constrictor	False	True	False	True	0	Yes
Chicken	True	True	False	False	2	No
Alligator	True	True	False	True	4	Yes
Dart frog	True	False	True	False	4	No

Current model:

- Has scales
- Cold blooded
- Has 0 or 4 legs

An Example

	Features					Label
Name	Egg-laying	Scales	Poisonous	Cold-blooded	# legs	Reptile
Cobra	True	True	True	True	0	Yes
Rattlesnake	True	True	True	True	0	Yes
Boa constrictor	False	True	False	True	0	Yes
Chicken	True	True	False	False	2	No
Alligator	True	True	False	True	4	Yes
Dart frog	True	False	True	False	4	No
Salmon	True	True	False	True	0	No
Python	True	True	False	True	0	Yes

Current model:

- Has scales
- Cold blooded
- Has 0 or 4 legs

No (easy) way to add to rule that will correctly classify salmon and python (since identical feature values)

An Example

	Features					Label
Name	Egg-laying	Scales	Poisonous	Cold-blooded	# legs	Reptile
Cobra	True	True	True	True	0	Yes
Rattlesnake	True	True	True	True	0	Yes
Boa constrictor	False	True	False	True	0	Yes
Chicken	True	True	False	False	2	No
Alligator	True	True	False	True	4	Yes
Dart frog	True	False	True	False	4	No
Salmon	True	True	False	True	0	No
Python	True	True	False	True	0	Yes

Good model:

- Has scales
- Cold blooded

Not perfect, but no false negatives (anything classified as not reptile is correctly labeled); some false positives (may incorrectly label some animals as reptile)

Need to Measure Distances between Features

- Feature engineering:
  - Deciding which features to include and which are merely adding noise to classifier
  - Defining how to measure distances between training examples (and ultimately between classifiers and new instances)
  - Deciding how to weight relative importance of different dimensions of feature vector, which impacts definitionof distance

Measuring Distance Between Animals

- We can think of our animal examples as consisting of four binary features and one integer feature
- One way to learn to separate reptiles from non-reptiles is to measure the distance between pairs of examples, and use that:
  - To cluster nearby examples into a common class (unlabeled data), or
  - To find a classifier surface in space of examples that optimally separates different (labeled) collections of examples from other collections

```
rattlesnake = [1,1,1,1,0]
boa constrictor = [0,1,0,1,0]
dart Frog = [1,0,1,0,4]
```

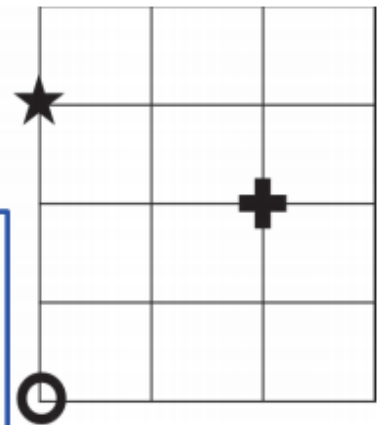
Can convert examples into feature vectors

Minkowski Metric

$$dist(X1, X2, p) = \left(\sum_{k=1}^{len} abs(X1_k - X2_k)^p\right)^{1/p}$$

p = 1: Manhattan Distance
p = 2: Euclidean Distance

Need to measure distances between feature vectors

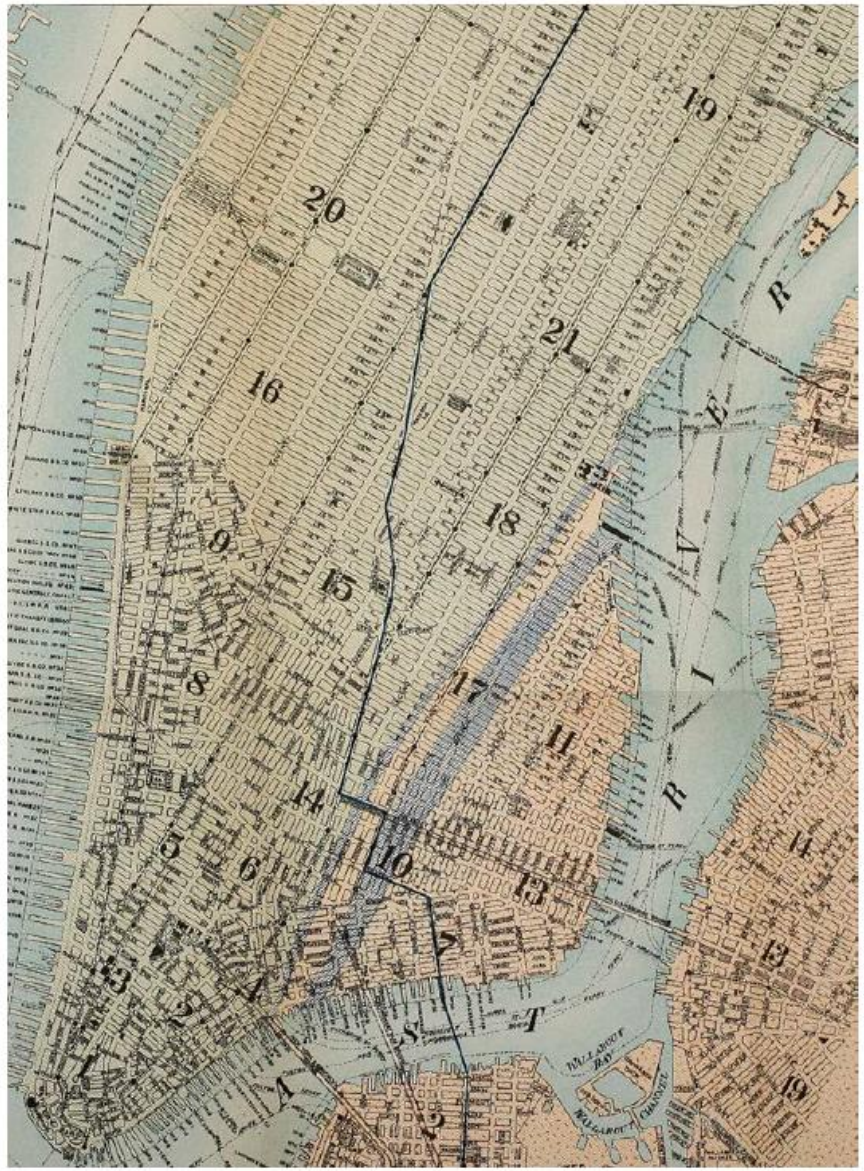


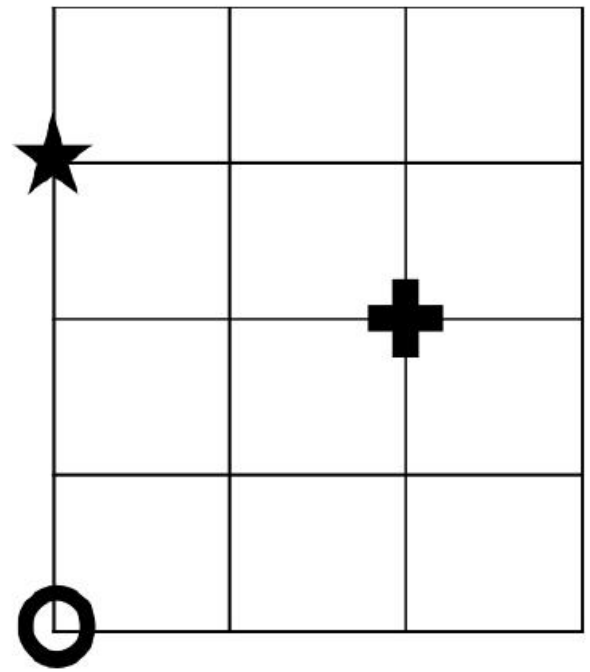
Typically use Euclidean metric; Manhattan may be appropriate if different dimensions are not comparable

Is circle closer to star or cross?

- Euclidean distance
  - Cross – 2.8
  - Star – 3
- Manhattan Distance
  - Cross – 4
  - Star - 3

Manhattan (1902)





```
def minkowskiDist(v1, v2, p):
    """Assumes v1 and v2 are equal-length arrays of numbers
       Returns Minkowski distance of order p between v1 and v2"""
    dist = 0.0
    for i in range(len(v1)):
        dist += abs(v1[i] - v2[i])**p
    return dist**(1.0/p)
```

```
class Animal(object):
    def __init__(self, name, features):
        """Assumes name a string; features a list of numbers"""
        self.name = name
        self.features = pylab.array(features)

    def getName(self):
        return self.name

    def getFeatures(self):
        return self.features

    def distance(self, other):
        """Assumes other an Animal
           Returns the Euclidean distance between feature vectors
              of self and other"""
        return minkowskiDist(self.getFeatures(),
                             other.getFeatures(), 2)
```

Euclidean Distance Between Animals

```
rattlesnake = [1,1,1,1,0]
boa constrictor = [0,1,0,1,0]
dartFrog = [1,0,1,0,4]
```

Euclidean Distance Between Animals

```
rattlesnake = [1,1,1,1,0]
boa constrictor = [0,1,0,1,0]
dartFrog = [1,0,1,0,4]
```

	rattlesnake	boa constrictor	dart frog
rattlesnake	--	1.414	4.243
boa constrictor	1.414	--	4.472
dart frog	4.243	4.472	--

Using Euclidean distance, rattlesnake and boa constrictor are much closer to each other, than they are to the dart frog

Add an Alligator

- `alligator = Animal('alligator', [1,1,0,1,4])`
- `animals.append(alligator)`
- `compareAnimals(animals, 3)`

Add an Alligator

```
alligator = Animal('alligator', [1,1,0,1,4])
animals.append(alligator)
compareAnimals(animals, 3)
```

	rattlesnake	boa constrictor	dart frog	alligator
rattlesnake	--	1.414	4.243	4.123
boa constrictor	1.414	--	4.472	4.123
dart frog	4.243	4.472	--	1.732
alligator	4.123	4.123	1.732	--

Alligator is closer to dart frog than to snakes – why?

- Alligator differs from frog in 3 features, from boa in only 2 features
- But scale on “legs” is from 0 to 4, on other features is 0 to 1
- “legs” dimension is disproportionately large

Using Binary Features

```
rattlesnake = [1,1,1,1,0]
boa constrictor = [0,1,0,1,0]
dartFrog = [1,0,1,0,1]
Alligator = [1,1,0,1,1]
```

	rattlesnake	boa constrictor	dart frog	alligator
rattlesnake	--	1.414	1.732	1.414
boa constrictor	1.414	--	2.236	1.414
dart frog	1.732	2.236	--	1.732
alligator	1.414	1.414	1.732	--

Now alligator is closer to snakes than it is to dart frog – makes more sense

Feature Engineering Matters

Producing the Distance Matrix

```
columnLabels = []
for a in animals:
    columnLabels.append(a.getName())
rowLabels = columnLabels[:]
tableVals = []
#Get distances between pairs of animals
#For each row
for a1 in animals:
    row = []
    #For each column
    for a2 in animals:
        if a1 == a2:
            row.append('--')
        else:
            distance = a1.distance(a2)
            row.append(str(round(distance, precision)))
    tableVals.append(row)
```

Producing the Table

```
#Produce table
    table = pylab.table(rowLabels = rowLabels,
                        colLabels = columnLabels,
                        cellText = tableVals,
                        cellLoc = 'center',
                        loc = 'center',
                        colWidths = [0.138]*len(animals))
    table.auto_set_font_size(False)
    table.set_fontsize(10)
    table.scale(1, 2.5)
    pylab.axis('off')
    pylab.savefig('distances')
```

Supervised versus Unsupervised Learning

- When given unlabeled data, try to find clusters of examples near each other
  - Use centroids of clusters as definition of each learned class
  - New data assigned to closest cluster
- When given labeled data, learn mathematical surface that "best" separates labeled examples, subject to constraints on complexity of surface (don't over fit)
  - New data assigned to class based on portion of feature space carved out by classifier surface in which it lies

Issues of Concern When Learning Models

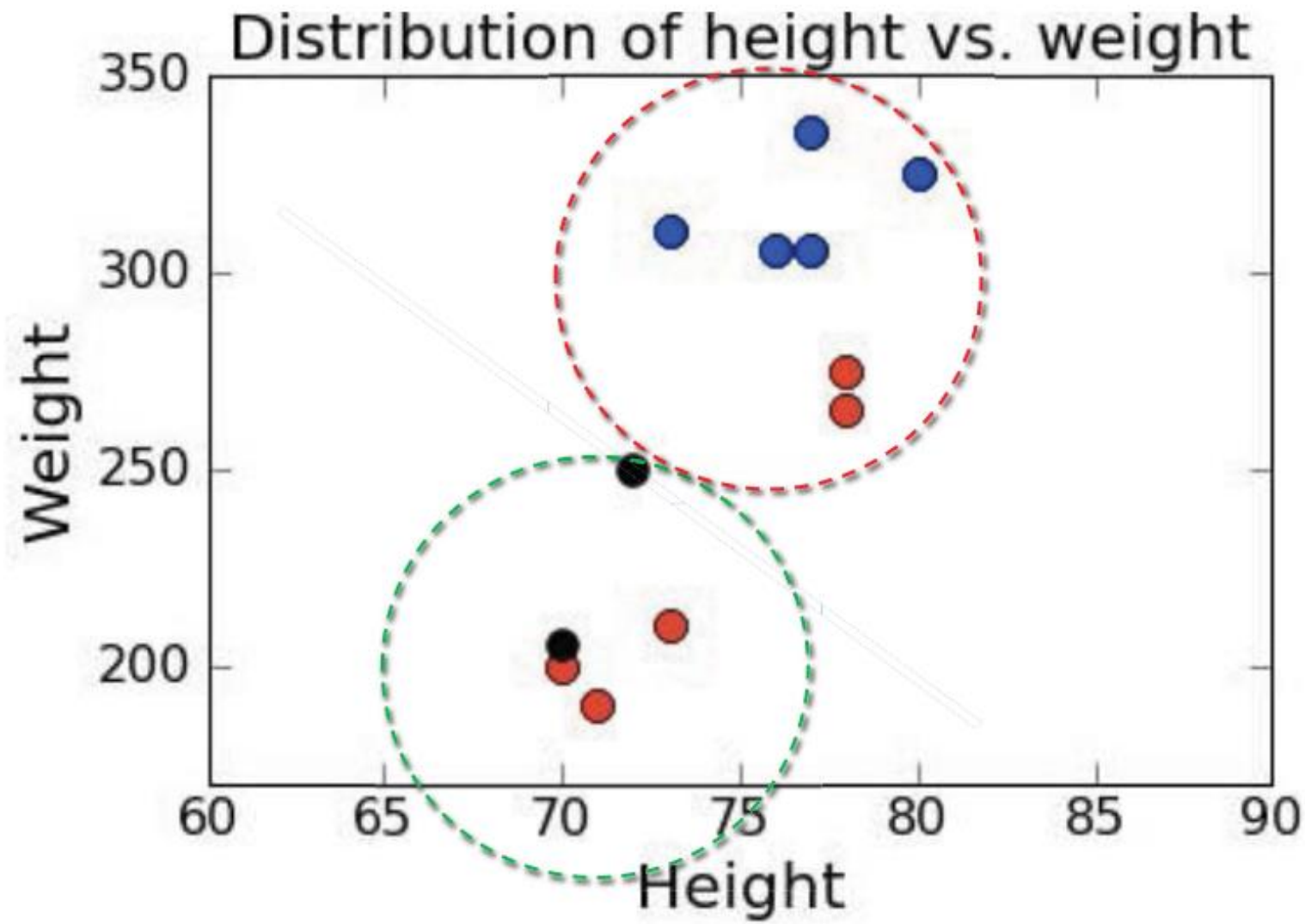
Learned models will depend on:

- Distance metric between examples
- Choice of feature vectors
- Constraints on complexity of model
  - Specified number of clusters
  - Complexity of separating surface
  - Want to avoid over fitting problem (each example is its own cluster, or a complex separating surface)

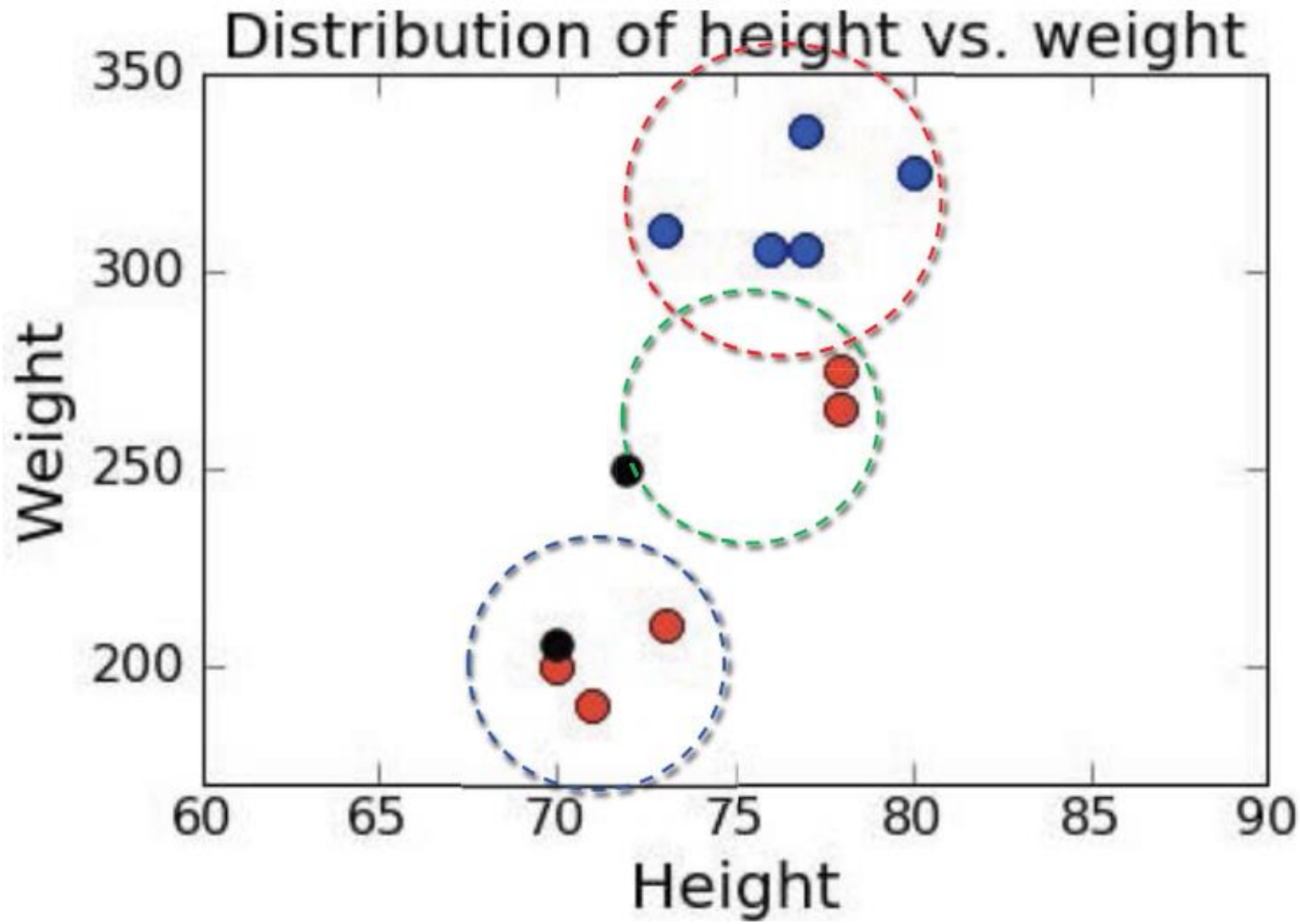
Clustering approaches

- Suppose we know that there are k different groups in our training data, but don't know labels
  - Pick k samples (at random?) as exemplars
  - Cluster remaining samples by minimizing distance between samples in same cluster (objective function) – put sample in group with closest exemplar
  - Find median example in each cluster as new exemplar
  - Repeat until no change
- Issues:
  - How do we decide on the best number of clusters?
  - How do we select the best features, the best distance metric?

Clustering using Unlabeled Data



Fitting Three Clusters Unsupervised



Classification approaches

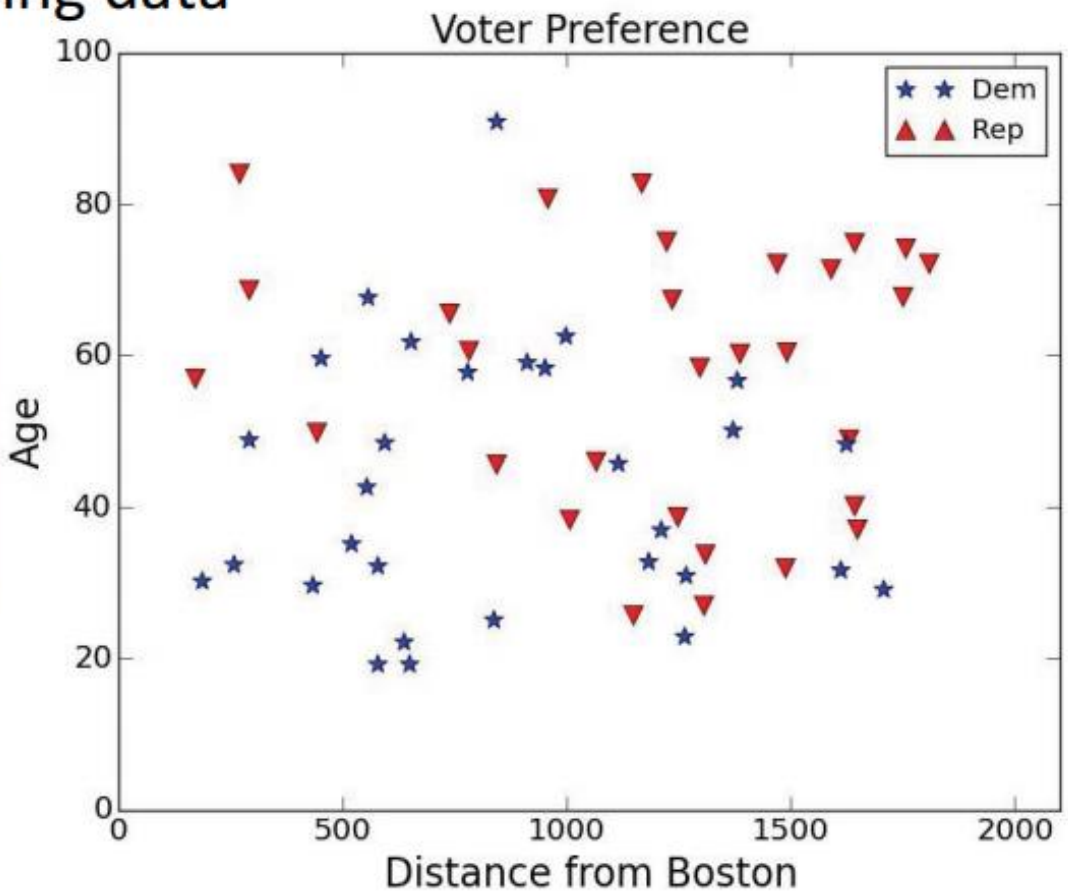
- Want to find boundaries in feature space that separate different classes of labeled examples
  - Look for simple surface (e.g. best line or plane) that separates classes
  - Look for more complex surfaces (subject to constraints) that separate classes
  - Use voting schemes
    - Find k nearest training examples, use majority vote to select label

- Issues:
  - How do we avoid over-fitting to data?
  - How do we measure performance?
  - How do we select best features?

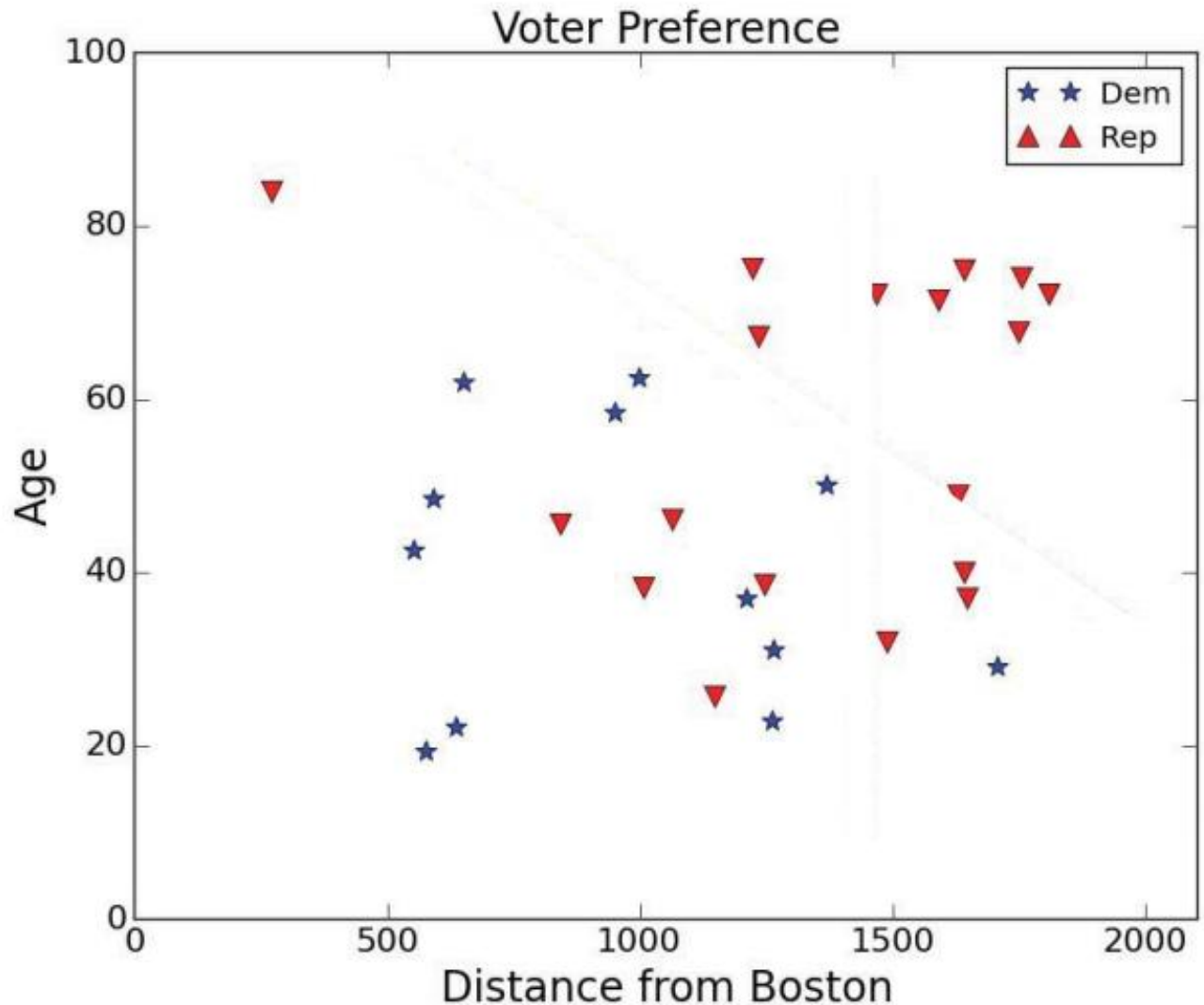
Classification

- Attempt to minimize error on training data
  - Similar to fitting a curve to data
- Evaluate on training data

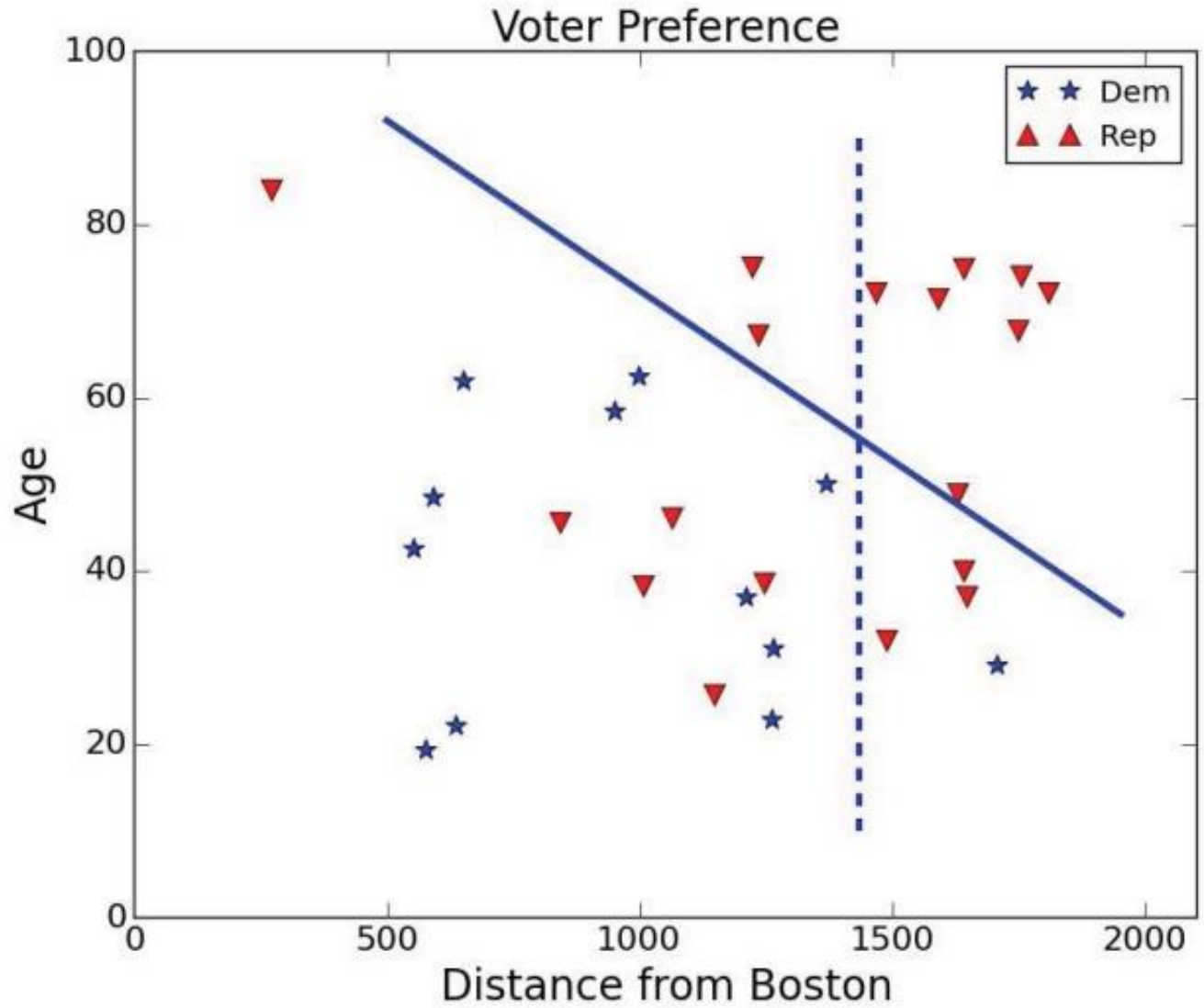
Voter preference, by age and distance from Boston



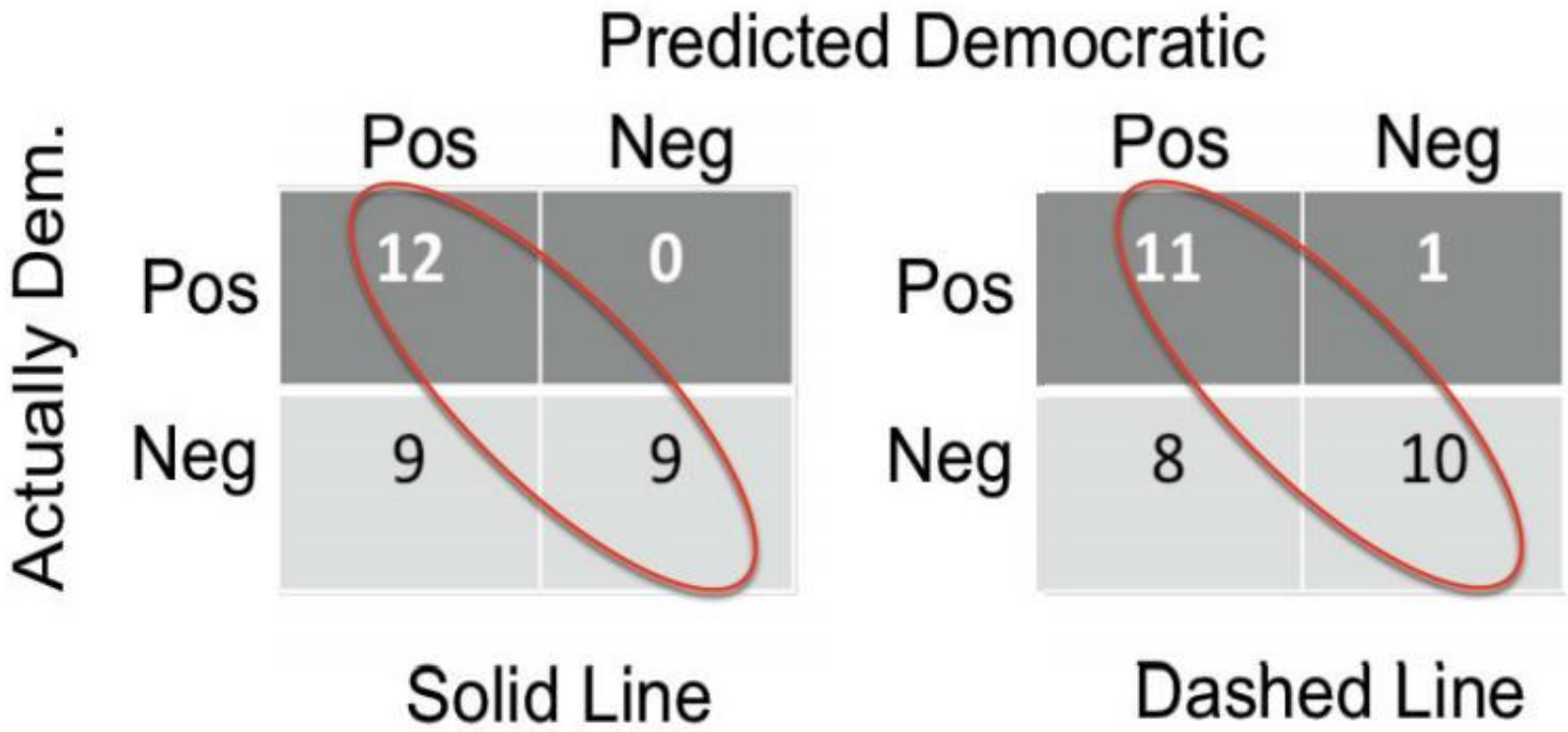
Randomly Divide Data into Training and Test Set



Two Possible Models for a Training Set



Confusion Matrices (Training Error)

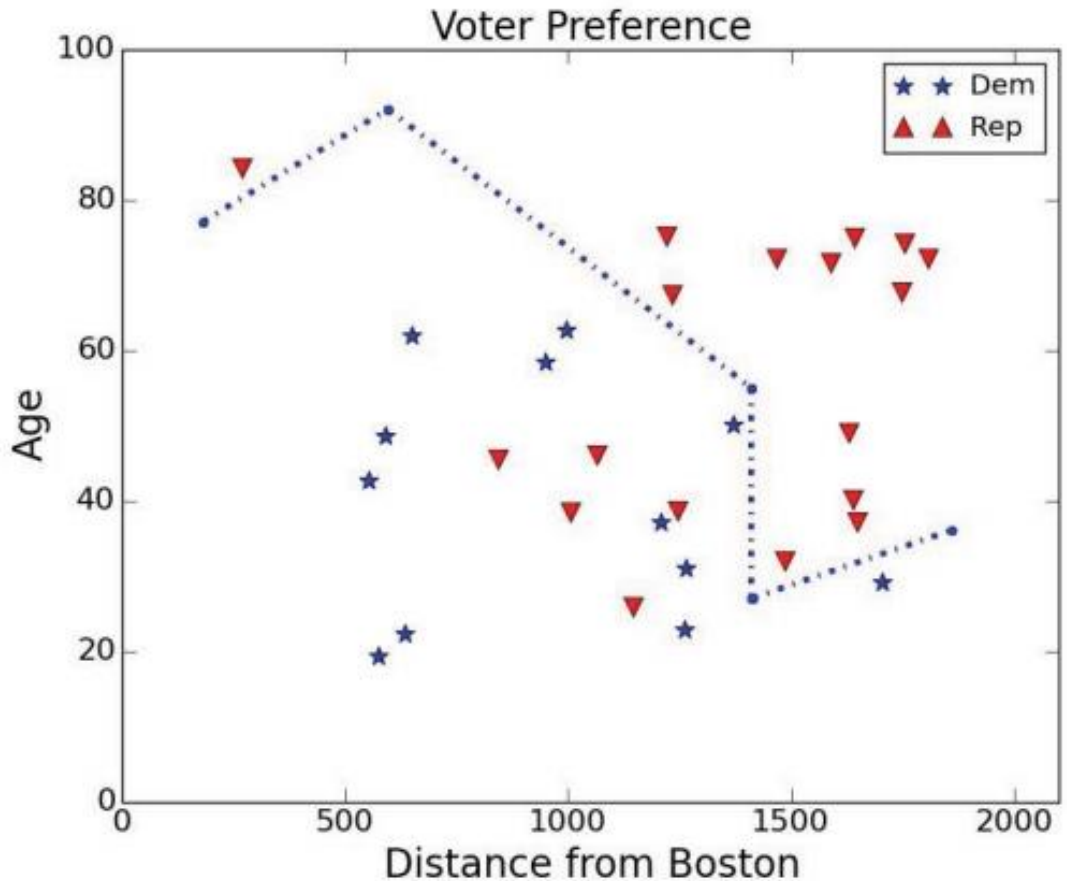


Training Accuracy of Models

$$accuracy = \frac{true\ positive + true\ negative}{true\ positive + true\ negative + false\ positive + false\ negative}$$

- 0.7 for both models
  - Which is better?
- Can we find a model with less training error?

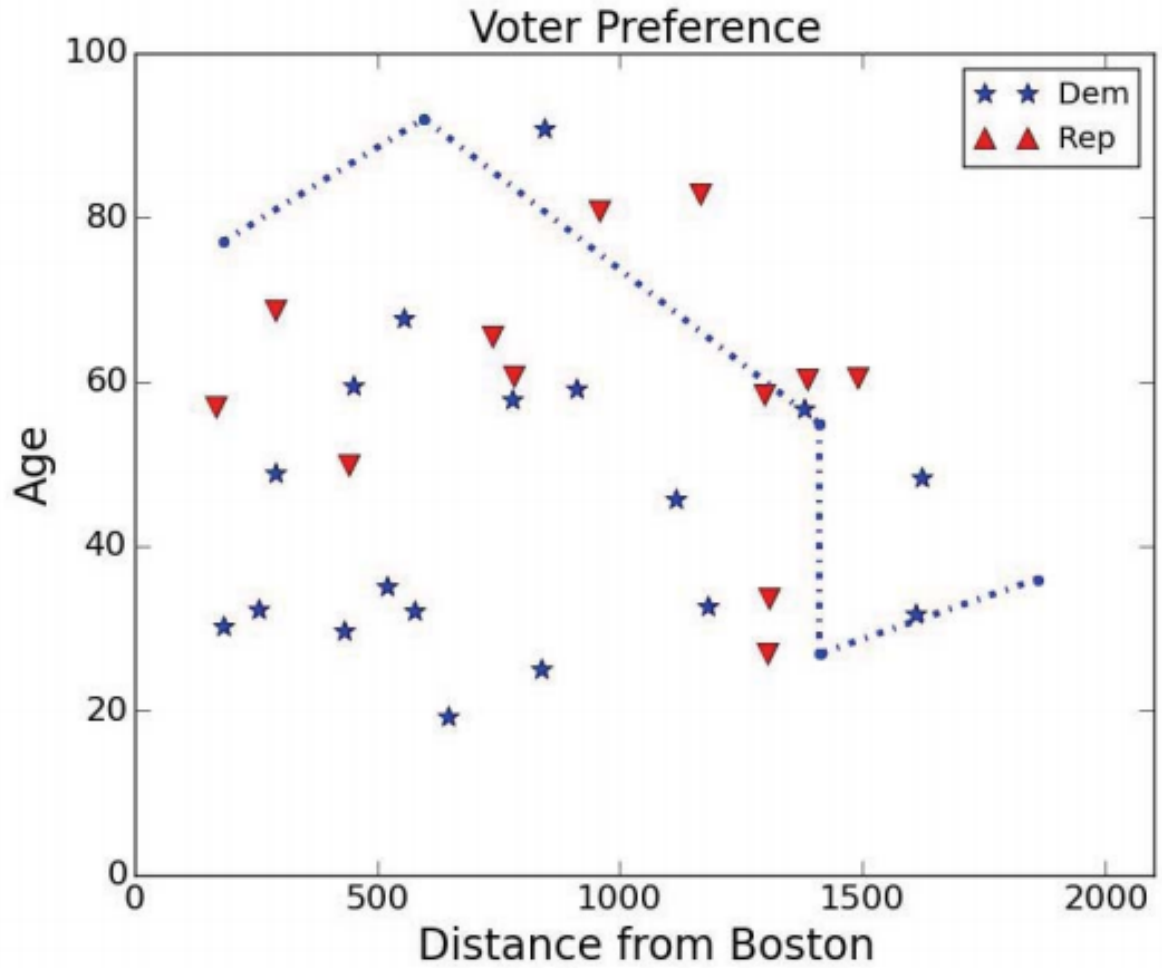
A More Complex Model



TP = 12, FP = 5, TN = 13, FN = 0

Accuracy = 25/30 = 0.833

Applying Model to Test Data



TP = 14, FP = 4, TN = 4, FN = 8

Accuracy = 18/30 = 0.6

Other Statistical Measures

$$positive\ predictive\ value = \frac{true\ positive}{true\ positive + false\ positive}$$

- Solid line model: .57
- Dashed line model: .58
- Complex model, training: .71
- Complex model, testing: .78

- You will also see "sensitivity" versus "specificity"

$$sensitivity = \frac{true\ positive}{true\ positive + false\ negative}$$

$$specificity = \frac{true\ negative}{true\ negative + false\ positive}$$

Percentage correctly found
Percentage correctly rejected

Summary

- Machine learning methods provide a way of building models of processes from data sets
  - Supervised learning uses labeled data, and creates classifiers that optimally separate data into known classes
  - Unsupervised learning tries to infer latent variables by clustering training examples into nearby groups
- Choice of features influences results
- Choice of distance measurement between examples influences results
- We will see some examples of clustering methods, such as k-means
- We will see some examples of classifiers, such as k nearest neighbor methods

To Do.

- Assignment 11
- Assignment – Assessing the Model
- Articles to read:
  - https://developers.google.com/machine-learning/data-prep/transform/normalization
  - https://keytodatascience.com/confusion-matrix/
  - https://blogs.oracle.com/ai-and-datascience/post/a-simple-guide-to-building-a-confusion-matrix

- before you leave the lab, decide on FSR or FE
- Quiz 4 (24th May 2022)