Welcome to the course!

UNSUPERVISED LEARNING IN R

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Chapter 1 overview

- Unsupervised learning
- Three major types of machine learning
- Execute one type of unsupervised learning using R

Types of machine learning

- Unsupervised learning
  - Finding structure in unlabeled data
- Supervised learning
  - Making predictions based on labeled data
  - Predictions like regression or classification
- Reinforcement learning

Labeled vs. unlabeled data

Features

Observations

Color	Shape	Size
Blue	Square	10
Red	Ellipse	2.4
Red	Ellipse	20.7

Unlabeled data

[1] Sample from Murphy, Machine Learning: A Probabilistic Perspective

Labeled vs. unlabeled data

Features

Observations

Color	Shape	Size	Label
Blue	Square	10	1
Red	Ellipse	2.4	1
Red	Ellipse	20.7	2

Labeled data

[1] Sample from Murphy, Machine Learning: A Probabilistic Perspective

Unsupervised learning - clustering

- Finding homogeneous subgroups within larger group

People have features such as income, education attainment, and gender

Unsupervised learning - clustering

- Finding homogeneous subgroups within larger group

Unsupervised learning - clustering

- Finding homogeneous subgroups within larger group

Clustering

Clustering examples

Clustering examples

Unsupervised learning - dimensionality reduction

- Finding homogeneous subgroups within larger group
  - Clustering
- Finding patterns in the features of the data
  - Dimensionality reduction

Unsupervised learning - dimensionality reduction

- Find patterns in the features of the data
- Visualization of high dimensional data
- Pre-processing before supervised learning

Challenges and benefits

- No single goal of analysis
- Requires more creativity
- Much more unlabeled data available than cleanly labeled data

Let's practice!

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Introduction to k-means clustering

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k-means clustering algorithm

- First of two clustering algorithms covered in this course
- Breaks observations into pre-defined number of clusters

k-means in R

```
# k-means algorithm with 5 centers, run 20 times
kmeans(x, centers = 5, nstart = 20)
```

- One observation per row, one feature per column
- k-means has a random component
- Run algorithm multiple times to improve odds of the best model

First exercises

- First exercise uses synthetic data
- Synthetic data generated from 3 subgroups
- Selecting the best number of subgroups for k-means
- Example with more fun data later in the chapter

Let's practice!

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How k-means works and practical matters

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Objectives

- Explain how k-means algorithm is implemented visually
- Model selection: determining number of clusters

Observations
2
1
0
-1
-2
-2
-1
0
1
2

Random Cluster Assignment

Cluster Centers Calculated

Iteration 1 - After Reassignment

Iteration 2
2
1
0
-1
-2
-2
-1
0
1
2

Iteration 3
2
1
0
-1
-2
-2
-1
0
1
2

Iteration 4
2
1
0
-1
-2
-2
-1
0
1
2

Iteration 5
2
1
0
-1
-2
-2
-1
0
1
2

Model selection

- Recall k-means has a random component
- Best outcome is based on total within cluster sum of squares:
  - For each cluster
    - For each observation in the cluster
      - Determine squared distance from observation to cluster center
    - Sum all of them together

Model selection

```
# k-means algorithm with 5 centers, run 20 times
kmeans(x, centers = 5, nstart = 20)
```

- Running algorithm multiple times helps find the global minimum total within cluster sum of squares
- You'll see an example in the exercises

Identical groupings and Total Within SS, but different cluster labels

Determining the best number of clusters

- Trial and error is not the best approach

Determining the best number of clusters

- Trial and error is not the best approach

Let's practice!

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Introduction to the Pokemon data

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"Real" data exercise

The Pokemon dataset

```
head(pokemon)
```

	HitPoints	Attack	Defense	SpecialAttack	SpecialDefense	Speed
[1,]	45	49	49	65	65	45
[2,]	60	62	63	80	80	60
[3,]	80	82	83	100	100	80
[4,]	80	100	123	122	120	80
[5,]	39	52	43	60	50	65
[6,]	58	64	58	80	65	80

[1] https://www.kaggle.com/abcsds/pokemon [2] https://pokemondb.net/pokedex

Data challenges

- Selecting the variables to cluster upon
- Scaling the data (will handle in last chapter)
- Determining the number of clusters
  - Often no clean "elbow" in scree plot
  - This will be a core part of the exercises
- Visualize the results for interpretation

Let's practice!

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Review of k-means clustering

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Chapter review

- Unsupervised vs. supervised learning
- How to create k-means cluster model in R
- How k-means algorithm works
- Model selection
- Application to "real" (and hopefully fun) dataset

Coming up: chapter 2

Coming up: chapter 3

Coming up: chapter 4

```
# Repeat for components 1 and 3
plot(wisc.pr$x[, c(1, 3)], col = (diagnosis + 1),
       xlab = "PC1", ylab = "PC3")
```

See you in the next chapter!

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