CSCE 580: Introduction to AI
CSCE 581: Trusted AI

Lecture 18: Explanation, Machine Learning – Unsupervised

PROF. BIPLAV SRIVASTAVA, AI INSTITUTE

26TH OCT 2023

Carolinian Creed: "I will practice personal and academic integrity."

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Organization of Lecture 18

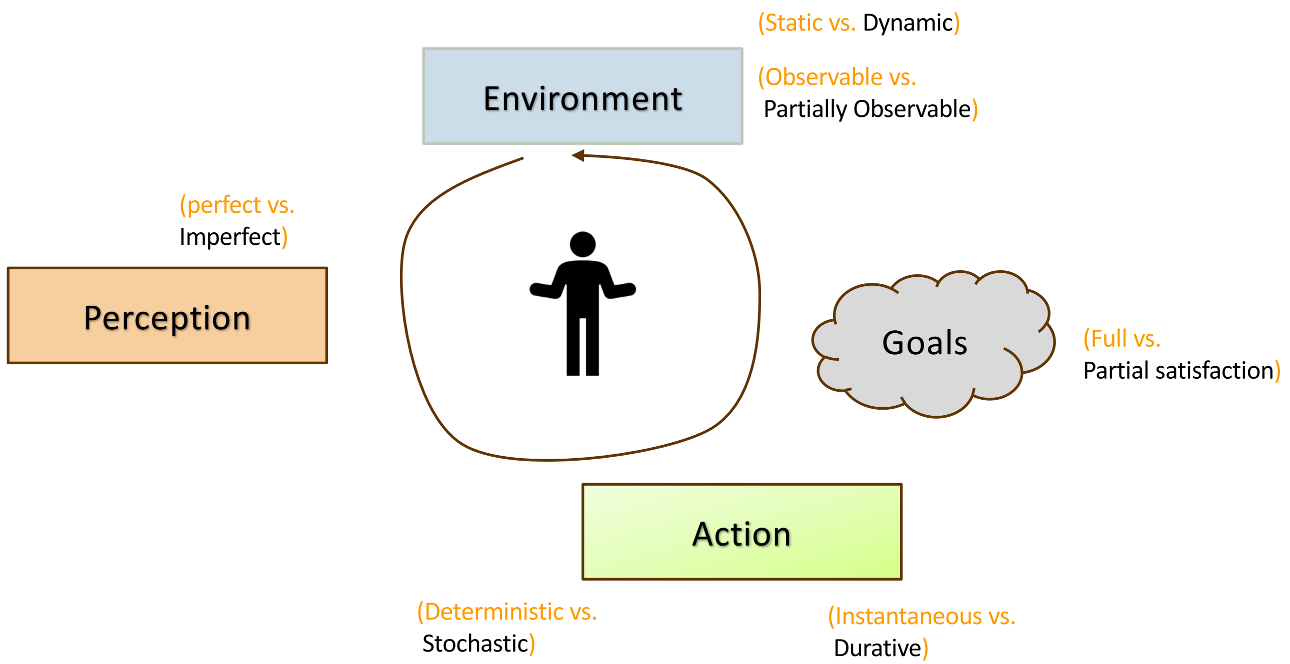
- Introduction Segment
  - Recap of Lecture 17
- Main Segment
  - Trust/ Explanations, LIME - Recap
  - Unsupervised ML
  - Algorithms
- Concluding Segment
  - Course Project Discussion
  - Quiz 3
  - About Next Lecture – Lecture 19
  - Ask me anything

Introduction Section

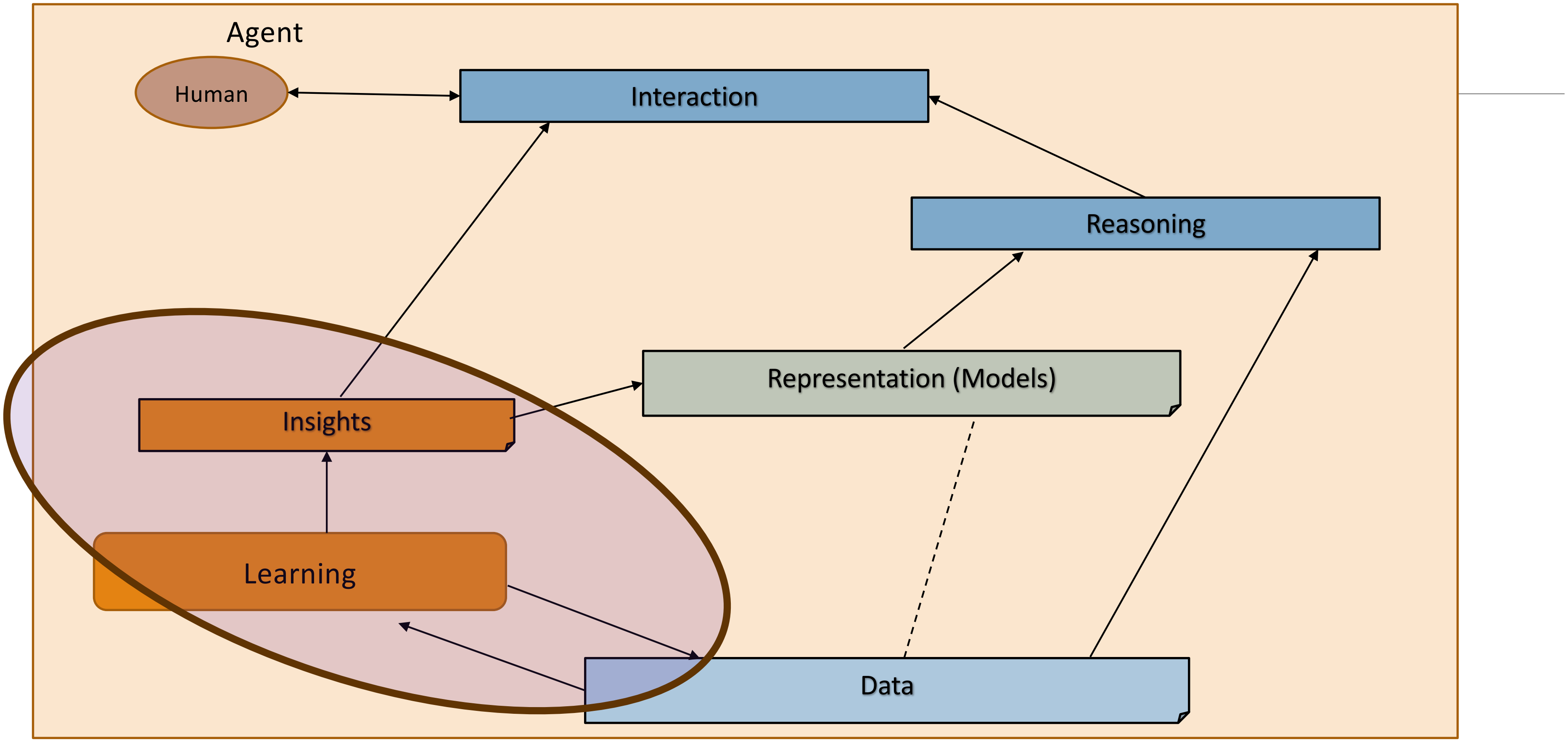
Recap of Lecture 17

- Topic discussed
  - Building Chatbots
  - Rasa
  - SafeChat Framework

Intelligent Agent Model



Relationship Between Main AI Topics



Where We Are in the Course

CSCE 580/ 581 – In This Course

- Week 1: Introduction, Aim: Chatbot / Intelligence Agent
- Weeks 2-3: Data: Formats, Representation and the Trust Problem
- Week 4-5: Search, Heuristics - Decision Making
- Week 6: Constraints, Optimization – Decision Making
- Week 7: Classical Machine Learning – Decision Making, Explanation
- Week 8: Machine Learning - Classification
- Week 9: Machine Learning - Classification – Trust Issues and Mitigation Methods
- Topic 10: Learning neural network, deep learning, Adversarial attacks
- Week 11: Large Language Models – Representation, Issues
- Topic 12: Markov Decision Processes, Hidden Markov models - Decision making
- Topic 13: Planning, Reinforcement Learning – Sequential decision making
- Week 14: AI for Real World: Tools, Emerging Standards and Laws; Safe AI/ Chatbots

Main Section

Credit: Retrieved from internet

Recap: AI Trust/ Explanations

Types of Explanations

- **Feature-based**: from the features of the data, which feature(s) were most important for given decision output
  - Example: For a loan, is it income or the person’s age ?
- **Sample-based**: from data in training, which data points were important for given test point; helps understand sampling and its representation in wider population
  - Example: For a loan, what instances similar to the loan application would have gotten the loan ?
- **Counter-factual**: what-ifs – what do you change about the input to change the decision output
  - Example: For a loan, does getting an additional borrower insurance increase chance of getting the loan?
- Natural language

Source: Explainable Machine Learning in Deployment, FAT* 2020

Explanation Taxonomy

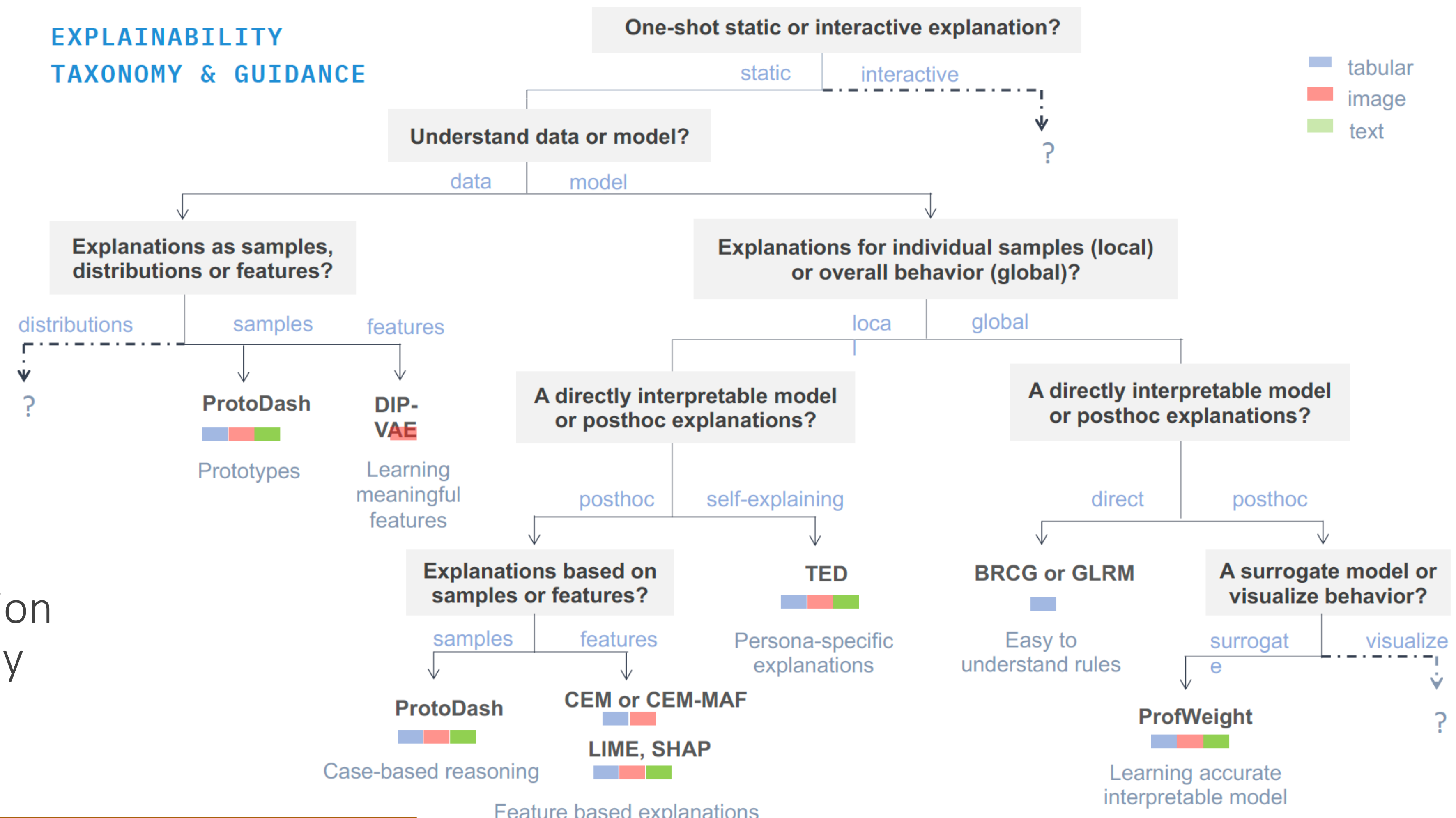


Figure Credit: Diptikalyan Saha and Vijay Arya, Oct 2021

Source: Fairness and Machine Learning by Solon Barocas, Moritz Hardt, Arvind Narayanan (https://www.fairmlbook.org)

A Step Towards Fairness

Broad classes

- **Individual fairness**: similar individuals to be treated similarly
- **Group fairness**: statistical property of decision as a group should be representative of the population
- ***Both* individual and group fairness, and use a single metric**: generalized entropy index

Guidance: ***Selection of metric is application driven***

Name	Closest relative	Note	Reference
Statistical parity	Independence	Equivalent	Dwork et al. (2011)
Group fairness	Independence	Equivalent	
Demographic parity	Independence	Equivalent	
Conditional statistical parity	Independence	Relaxation	Corbett-Davies et al. (2017)
Darlington criterion (4)	Independence	Equivalent	Darlington (1971)
Equal opportunity	Separation	Relaxation	Hardt, Price, Srebro (2016)
Equalized odds	Separation	Equivalent	Hardt, Price, Srebro (2016)
Conditional procedure accuracy	Separation	Equivalent	Berk et al. (2017)
Avoiding disparate mistreatment	Separation	Equivalent	Zafar et al. (2017)
Balance for the negative class	Separation	Relaxation	Kleinberg, Mullainathan, Raghavan (2016)
Balance for the positive class	Separation	Relaxation	Kleinberg, Mullainathan, Raghavan (2016)
Predictive equality	Separation	Relaxation	Chouldechova (2016)
Equalized correlations	Separation	Relaxation	Woodworth (2017)
Darlington criterion (3)	Separation	Relaxation	Darlington (1971)
Cleary model	Sufficiency	Equivalent	Cleary (1966)
Conditional use accuracy	Sufficiency	Equivalent	Berk et al. (2017)
Predictive parity	Sufficiency	Relaxation	Chouldechova (2016)
Calibration within groups	Sufficiency	Equivalent	Chouldechova (2016)
Darlington criterion (1), (2)	Sufficiency	Relaxation	Darlington (1971)

Machine Learning – Insights from Data

- Descriptive analysis
  - Describe a past phenomenon
  - **Methods**: classification (feedback from label), clustering, dimensionality reduction, anomaly detection, neural methods, reinforcement learning (feedback from hint/ reward)
- Predictive analysis
  - Predict about a new situation
  - **Methods**: time-series, neural networks
- Prescriptive analysis
  - What an agent should do
  - **Methods**: simulation, reinforcement learning, reasoning
- New areas
  - Counterfactual analysis
  - Causal Inferencing
  - Scenario planning

Unsupervised Machine Learning

- Group data into clusters/ classes without supervision
  - Limited supervision

- What is a good cluster ?
  - Samples within a cluster should be "**near**" to each other (**cohesiveness**)
  - Samples in a cluster should be "**far**" from other samples in other clusters. (**distinctiveness**)

Data Representation

- Data matrix representation
  - N objects (data rows) x p attributes (columns)
  - Similar to classification

- Dissimilarity matrix
  - Object x Object structure
  - D(I, j) is difference or dissimilarity between (I, j), 0 means similar and 1 means dissimilar

Clustering for Data Understanding and Applications

- Biology: taxonomy of living things: kingdom, phylum, class, order, family, genus and species
- Information retrieval: document clustering
- Land use: Identification of areas of similar land use in an earth observation database
- Marketing: Help marketers discover distinct groups in their customer bases, and then use this knowledge to develop targeted marketing programs
- City-planning: Identifying groups of houses according to their house type, value, and geographical location
- Earth-quake studies: Observed earth quake epicenters should be clustered along continent faults
- Climate: understanding earth climate, find patterns of atmospheric and ocean
- Economic Science: market resarch

Content: Jiawei Han, Micheline Kamber and Jian Pei Data Mining: Concepts and Techniques, 3rd ed.

Clustering as a Preprocessing Tool (Utility)

- Summarization:
  - Preprocessing for regression, PCA, classification, and association analysis
- Compression:
  - Image processing: vector quantization
- Finding K-nearest Neighbors
  - Localizing search to one or a small number of clusters
- Outlier detection
  - Outliers are often viewed as those “far away” from any cluster

Content: Jiawei Han, Micheline Kamber and Jian Pei
Data Mining: Concepts and Techniques, 3rd ed.

Considerations for a Clustering Algorithm

- Need a distance measure for ***far*** and ***near***
- Be able to explain what a cluster means
- Handle different types of attributes: numeric, categorical (nominal, ordinal), binary
- Detect different shapes of clusters
- Handle noisy data
- Scale
  - Size
  - Dimensions

Major Clustering Approaches (I)

Partitioning approach:

- Construct various partitions and then evaluate them by some criterion, e.g., minimizing the sum of square errors
- Typical methods: **k-means**, k-medoids, CLARANS

Hierarchical approach:

- Create a hierarchical decomposition of the set of data (or objects) using some criterion
- Typical methods: Diana, Agnes, **BIRCH**, CAMELEON

Density-based approach:

- Based on connectivity and density functions
- Typical methods: **DBSACN**, OPTICS, DenClue

Grid-based approach:

- based on a multiple-level granularity structure
- Typical methods: STING, WaveCluster, CLIQUE

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Major Clustering Approaches (II)

Model-based:

- A model is hypothesized for each of the clusters and tries to find the best fit of that model to each other
- Typical methods: **EM**, SOM, COBWEB

Frequent pattern-based:

- Based on the analysis of frequent patterns
- Typical methods: p-Cluster

User-guided or constraint-based:

- Clustering by considering user-specified or application-specific constraints
- Typical methods: COD (obstacles), constrained clustering

Link-based clustering:

- Objects are often linked together in various ways
- Massive links can be used to cluster objects: **SimRank**, LinkClus

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Partitioning Algorithms: Basic Concept

Partitioning method: Partitioning a database ***D*** of ***n*** objects into a set of ***k*** clusters, such that the sum of squared distances is minimized (where c_i is the centroid or medoid of cluster C_i)

$$E = \Sigma_{i=1}^{k} \Sigma_{p \in C_i} (p - c_i)^2$$

Given *k*, find a partition of *k clusters* that optimizes the chosen partitioning criterion

- Global optimal: exhaustively enumerate all partitions
- Heuristic methods: *k-means* and *k-medoids* algorithms
- *k-means* (MacQueen'67, Lloyd'57/'82): Each cluster is represented by the center of the cluster
- *k-medoids* or PAM (Partition around medoids) (Kaufman & Rousseeuw'87): Each cluster is represented by one of the objects in the cluster

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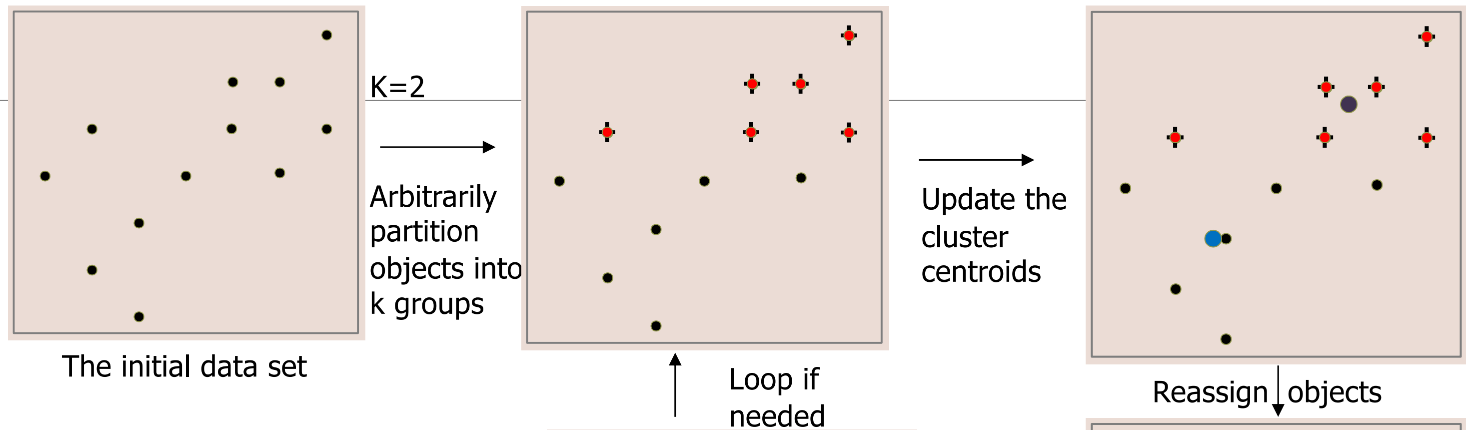
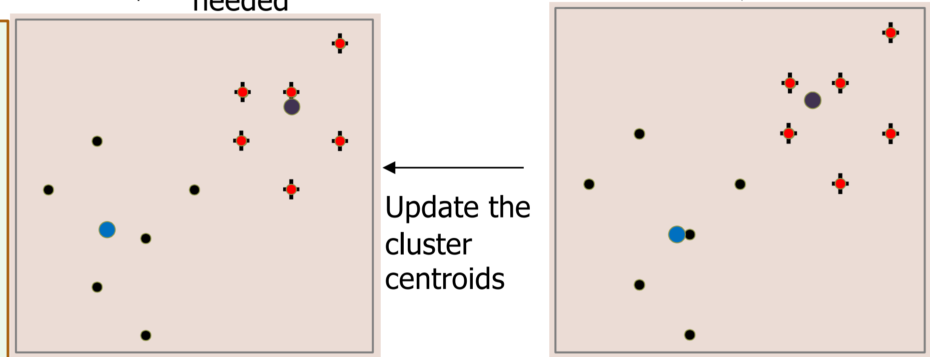
Data Mining: Concepts and Techniques, 3rd ed.

An Example of *K-Means* Clustering





- Partition objects into *k* nonempty subsets
- Repeat
  - Compute centroid (i.e., mean point) for each partition
  - Assign each object to the cluster of its nearest centroid
- Until no change

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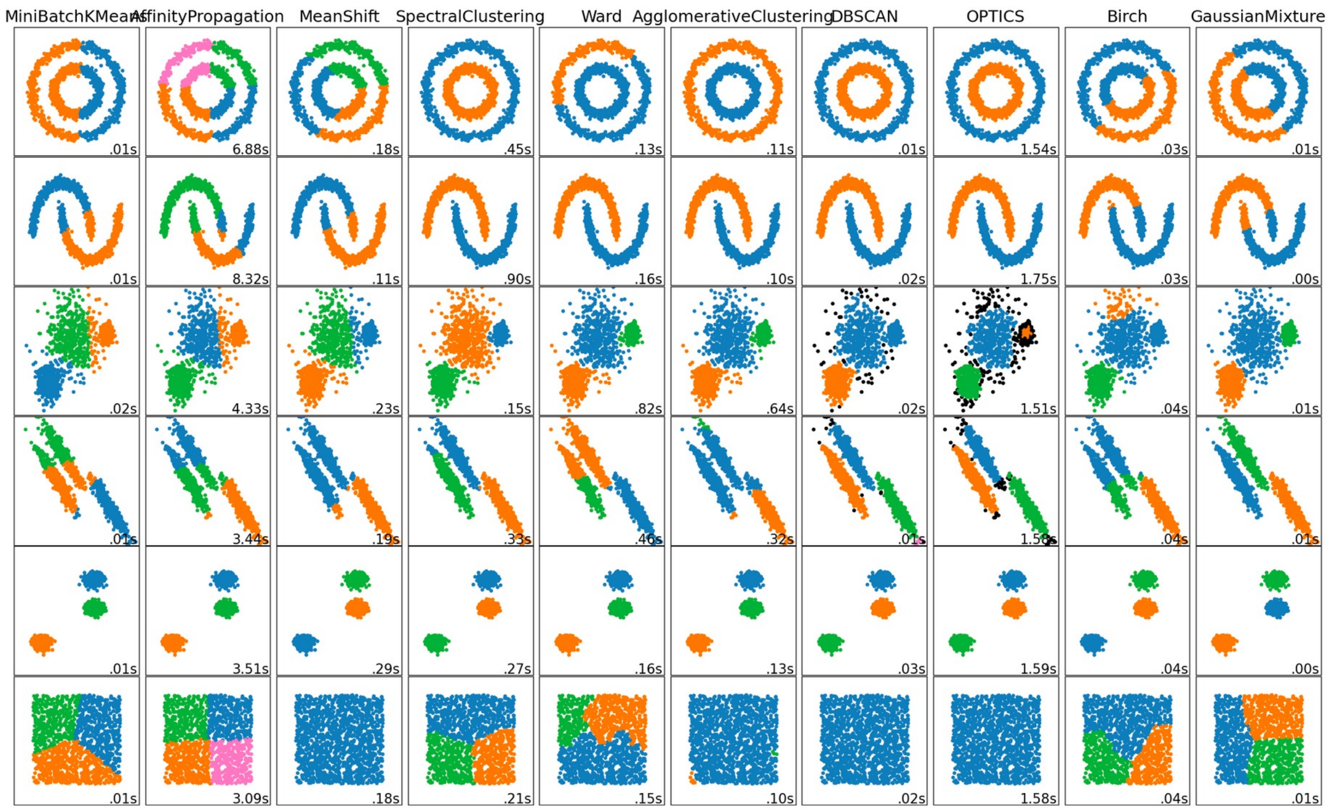
Comments on the *K-Means* Method

- **Strength**: *Efficient*: $O(tkn)$, where n is # objects, k is # clusters, and t is # iterations. Normally, k, t << n.
  - Comparing: PAM: $O(k(n-k)^2)$, CLARA: $O(ks^2 + k(n-k))$
- **Comment**: Often terminates at a *local optimal*.
- **Weakness**
  - Applicable only to objects in a continuous n-dimensional space
    - Using the k-modes method for categorical data
    - In comparison, k-medoids can be applied to a wide range of data
  - Need to specify *k, the number* of clusters, in advance (there are ways to automatically determine the best k (see Hastie et al., 2009)
  - Sensitive to noisy data and *outliers*
  - Not suitable to discover clusters with *non-convex shapes*

Exercise: Weka

- Use K-means on weather.arff
- Vary k

Snapshot of Clustering Methods



A comparison of the clustering algorithms in scikit-learn

Credit: https://scikit-learn.org/stable/modules/clustering.html

Snapshot of Clustering Methods

Method name	Parameters	Scalability	Usecase	Geometry (metric used)
K-Means	number of clusters	Very large n_samples, medium n_clusters with MiniBatch code	General-purpose, even cluster size, flat geometry, not too many clusters, inductive	Distances between points
Affinity propagation	damping, sample preference	Not scalable with n_samples	Many clusters, uneven cluster size, non-flat geometry, inductive	Graph distance (e.g. nearest-neighbor graph)
Mean-shift	bandwidth	Not scalable with n_samples	Many clusters, uneven cluster size, non-flat geometry, inductive	Distances between points
Spectral clustering	number of clusters	Medium n_samples, small n_clusters	Few clusters, even cluster size, non-flat geometry, transductive	Graph distance (e.g. nearest-neighbor graph)
Ward hierarchical clustering	number of clusters or distance threshold	Large n_samples and n_clusters	Many clusters, possibly connectivity constraints, transductive	Distances between points
Agglomerative clustering	number of clusters or distance threshold, linkage type, distance	Large n_samples and n_clusters	Many clusters, possibly connectivity constraints, non Euclidean distances, transductive	Any pairwise distance
DBSCAN	neighborhood size	Very large n_samples, medium n_clusters	Non-flat geometry, uneven cluster sizes, outlier removal, transductive	Distances between nearest points
HDBSCAN	minimum cluster membership, minimum point neighbors	large n_samples, medium n_clusters	Non-flat geometry, uneven cluster sizes, outlier removal, transductive, hierarchical, variable cluster density	Distances between nearest points
OPTICS	minimum cluster membership	Very large n_samples, large n_clusters	Non-flat geometry, uneven cluster sizes, variable cluster density, outlier removal, transductive	Distances between points
Gaussian mixtures	many	Not scalable	Flat geometry, good for density estimation, inductive	Mahalanobis distances to centers
BIRCH	branching factor, threshold, optional global clusterer.	Large n_clusters and n_samples	Large dataset, outlier removal, data reduction, inductive	Euclidean distance between points
Bisecting K-Means	number of clusters	Very large n_samples, medium n_clusters	General-purpose, even cluster size, flat geometry, no empty clusters, inductive, hierarchical	Distances between points

Credit: https://scikit-learn.org/stable/modules/clustering.html

Course Project

Project Discussion: What Problem Fascinates You ?

- Data
  - Water
  - Finance
  - …
- Analytics
  - Search, Optimization, Learning, Planning, …
- Application
  - Building chatbot
- Users
  - Diverse demographics
  - Diverse abilities
  - Multiple human languages

Project execution in sprints

- Sprint 1: (Sep 12 – Oct 5)
  - Solving: Choose a decision problem, identify data, work on solution methods
  - Human interaction: Develop a basic chatbot (no AI), no problem focus
- Sprint 2: (Oct 10 – Nov 9)
  - Solving: Evaluate your solution on problem
  - Human interaction: Integrated your choice of chatbot (rule-based or learning-based) and methods
- Sprint 3: (Nov 14 – 30)
  - **Evaluation:** Comparison of your solver chatbot with an LLM-based alternative, like ChatGPT

Project Discussion: Dates and Deliverables

Project execution in sprints

- Sprint 1: (Sep 12 – Oct 5)
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- Sprint 3: (Nov 14 – 30)
  - **Evaluation:** Comparison of your solver chatbot with an LLM-based alternative, like ChatGPT

- Oct 12, 2023
  - Project checkpoint
  - In-class presentation
- Nov 30, 2023
  - Project report due
- Dec 5 / 7, 2023
  - In-class presentation

Skeleton: A Basic Chatbot

- Run in an infinite loop until the user wants to quit
- Handle any user response
  - User can quit by typing “Quit” or “quit” or just “q”
  - User can enter any other text and the program has to handle it. The program should write back what the user entered and say – “I do not know this information”.
- Handle known user query types // Depends on your project
  - “Tell me about N-queens”, “What is N ?”
  - “Solve for N=4?”
  - “Why is this a solution? ”
- Handle chitchat // Support at least 5, extensible from a file
  - “Hi” => **“Hello”**
  - …
- ***Store session details in a file***

Illustrative Project

1. **Title**: Solve and explain solving of n-queens puzzle
2. **Key idea**: Show students how a course project will look like
3. **Who will care when done**: students of the course, prospective AI students and teachers
4. **Data need**: n: the size of game; interaction
5. **Methods**: search
6. **Evaluation**: correctness of solution, quality of explanation, appropriateness of chat
7. **Users**: with and without AI background; with and without chess background
8. **Trust issue**: user may not believe in the solution, may find interaction offensive (why queens, not kings? …)

Project Discussion: Illustration

1. Create a private Github repository called "CSCE58x-Fall2023-<studentname>-Repo". Share with Instructor (biplav-s) and TA (kausik-l)
2. Create Google folder called "CSCE58x-Fall2023-<studentname>-SharedInfo". Share with Instructor (prof.biplav@gmail.com) and TA (lakkarajukausik90@gmail.com)
3. Create a Google doc in your Google repo called "Project Plan" and have the following by next class (Sep 5, 2023)

1. **Title**: Solve and explain solving of n-queens puzzle
2. **Key idea**: Show students how a course project will look like
3. **Who will care when done**: students of the course, prospective AI students and teachers
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Project Illustration: N-Queens

- Sprint 1: (Sep 12 – Oct 5)
  - Solving: Choose a decision problem, identify data, work on solution methods
    - Method 1: Random solution
    - Method 2: Search – BFS
    - Method 3: Search - …
  - Human interaction: Develop a basic chatbot (no AI) as outlined
  - Deliverable
    - Code structure in Github
      - ./data
      - ./code
      - ./docs
      - ./test
    - Presentation: Make sprint presentation on Oct 12, 2023

Reference: Project Rubric

- **Project results** – 60%
  - Working system ? – 30%
  - Evaluation with results superior to baseline? – 20%
  - Considered related work? – 10%
- **Project efforts** – 40%
  - Project report – 20%
  - Project presentation (updates, final) – 20%

- **Bonus**
  - Challenge level of problem – 10%
  - Instructor discretion – 10%
- **Penalty**
  - Lack of timeliness as per announced policy (right) - up to 30%

Milestones and **Penalties**

- Oct 12, 2023
  - Project checkpoint
  - In-class presentation
  - **Penalty: presentation not ready by Oct 10, 2023 [-10%]**
- Nov 30, 2023
  - Project report due
  - **Project report not ready by date [-10%]**
- Dec 5 / 7, 2023
  - In-class presentation
  - **Project presentations not ready by Dec 4, 2023 [-10%]**

Quiz 3

Discussion on Quiz 3; due on Tuesday (Nov 2, 2023)

Lecture 18: Summary

- We talked about
  - Building Chatbots
  - Rasa
  - SafeChat Framework

Concluding Section

About Next Lecture – Lecture 19

Lecture 19: Machine Learning - NN, Deep Learning

- Neural Networks
- Deep Learning
- Trust Issues