Clustering

Finding clumps in data

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#MachineLearning

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Clustering Analysis

- Unsupervised learning
  - Discover hidden structures in data where we don't know the right answer upfront
- **Clustering**
  - Find a natural grouping in data such that items in the same cluster are more similar to each other than those from different clusters
- Some applications
  - Medicine: classify different types of tissues
  - Marketing: group similar products
  - Image segmentation, object recognition
  - Social network analysis
  - Crime analysis: "hot" spatial areas; similar crimes

k-Means Clustering

- Prototype-based algorithm
  - Each cluster is represented by a "prototype" data point
  - As opposed to density-based
- Algorithm
  - Select k – number of clusters
  - Randomly pick k samples as "initial centroids"
  - Repeat until convergence (change in centers < tolerance):
    - Assign each sample to the nearest (using a distance metric) centroid
    - Move the centroids to the center of the newly created clusters
- Advantages: fast, simple, good for "spherical" clusters
- Disadvantages: we need to specify k, doesn't work too well with overlapping or hierarchical clusters

k-Means Clustering (2)

- Objective function
  - Minimize the **cluster inertia** $J = \sum_{i=0}^{n} \min_{\mu_j \in C} ||x_i - \mu_j||^2$
    - Within-cluster sum of squared errors (Euclidean distances)
- Generating clusters
  - We can use `scikit-learn` to generate "blobs" (clusters)

```
from sklearn.datasets import make_blobs
attributes, clusters = make_blobs(cluster_std = 1)
plt.scatter(attributes[:, 0], attributes[:, 1], c = clusters)
```

  - Other options – "circles", "moons", etc.

```
from sklearn.datasets import make_blobs, make_circles,
  make_regression, make_s_curve, make_swiss_roll
# The last two are 3D – you can either plot them
# or see their projections using the x, y and z axes
```

Example: k-Means Clustering

- Generate several datasets
  - Blobs, circles, moons
- Apply k-means clustering to each dataset
- Display the original clusters and the clustering results
  - How do they differ? Can you explain why?

```
from sklearn.cluster import KMeans

attributes, clusters = make_blobs()
k_means = KMeans(3, init = "random")
assigned = k_means.fit_predict(attributes)
# Original, generated clusters
plt.scatter(attributes[:, 0], attributes[:, 1], c = clusters)
plt.show()
# Assigned clusters
plt.scatter(attributes[:, 0], attributes[:, 1], c = assigned)
plt.show()
```

k-Means++

- Random initial seed ⇒ may lead to poor performance
  - If the initial points aren't placed well enough or if the clusters are too "mixed"
- k-Means++ uses centers which are far away from each other
  - Instead of random initialization
- Algorithm
  - Choose the first centroid uniformly at random
  - To choose the next centroids, use a weighted probability distribution
    - Based on all currently selected centroids
    - Further away ⇒ greater probability
  - After all centroids have been initialized, proceed as usual

Example: k-Means++

- Generate several datasets
  - Blobs, circles, moons
- Apply k-Means++

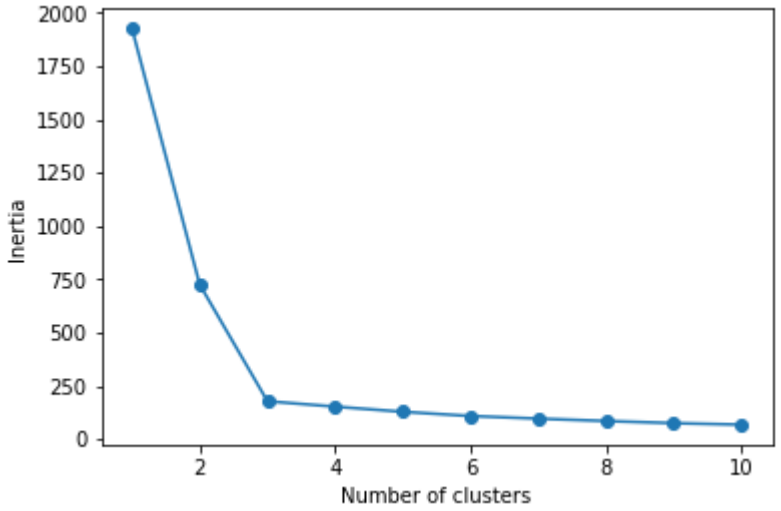
```
attributes, clusters = make_blobs()
k_means = KMeans(3, init = "k-means++")
assigned = k_means.fit_predict(attributes)
```

- Compare the performance of k-means++ versus k-means on blobs that are "close" to each other
  - Generate blobs with a higher standard deviation
  - Plot the centroids
  - * Count the misclassified points for the two algorithms

Finding an Optimal Number of Clusters

- **Elbow method** – graphical
- Inertia is a measure of clustering quality
  - Like grid search, initialize `KMeans` with a range of k values
  - Fit and calculate the inertia (given by default in `scikit-learn`)
  - Plot inertia vs. number of clusters
  - Find the "elbow point" of the plot – optimal
    - Inertia always decreases but some models overfit the data

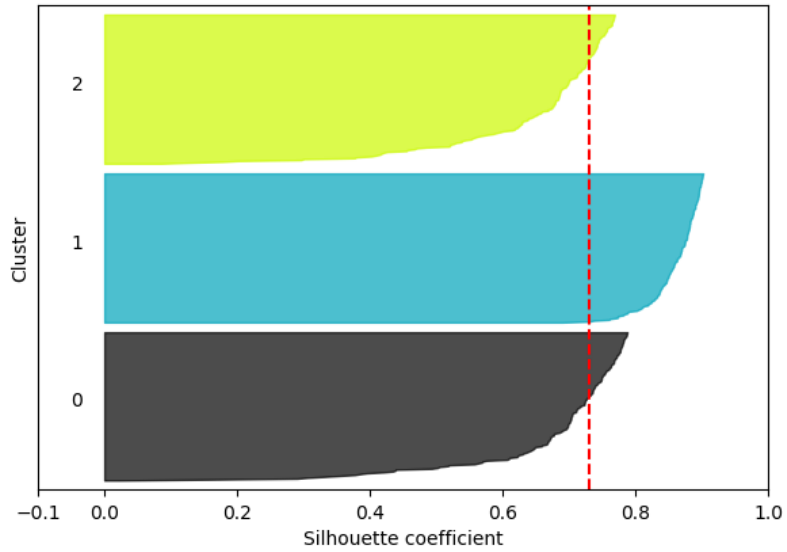
```
inertias = []
for i in range(1, 11):
  km = KMeans(n_clusters = i)
  km.fit(attributes)
  inertias.append(km.inertia_)
plt.plot(range(1,11), inertias, marker = "o")
plt.xlabel("Number of clusters")
plt.ylabel("Inertia")
plt.show()
```



Evaluating Clustering Quality

- **Silhouette analysis** – graphical
  - Use cluster cohesion (within-cluster distance) and cluster separation (between-cluster distance) to calculate the silhouette coefficient for each observation
    - $[-1;\ 1]$, 0 if the two distances are equal, 1 – ideal, -1 – worst
- Usage – import from `scikit-learn` and plot (example)

```
from sklearn.metrics import silhouette_samples
```



- Interpretation
  - Each color is a separate cluster
  - All silhouettes should be close to 1 (these are similar to bar charts)
  - All silhouettes have a similar "depth" and "width" (if they don't ⇒ suboptimal clustering)

Hierarchical Clustering

- Another prototype-based clustering
- Advantage – allows us to plot dendrograms
  - Visualizations of binary hierarchical clustering
  - Allow us to interpret the results
- Algorithm
  - Compute the distance matrix (distances between any two points)
  - Start with each point at its own cluster
  - Repeat until only one cluster is left:
    - Merge the two closest clusters and update the distances
    - Update the distance matrix
  - In `scikit-learn`, `linkage` describes the selected distance metric

```
from sklearn.cluster import AgglomerativeClustering
aggl = AgglomerativeClustering(n_clusters = 3, linkage = "complete")
```

Example: Hierarchical Clustering

- Perform hierarchical (agglomerative) clustering on several datasets and visualize the results
  - Blobs, moons, nested circles
  - Try different linkage strategies
- Plot a dendrogram
  - `linkage()` calculates a distance matrix
  - `dendrogram()` creates the plot (x-axis: ID, y-axis: distance)

```
from scipy.cluster.hierarchy import linkage, dendrogram
row_clusters = linkage(attributes, method = "complete", metric = "euclidean")
dendrogram(row_clusters, labels = clusters)
plt.show()

# Show only the last 10 merged clusters
dendrogram(row_clusters, labels = clusters, truncate_mode = "lastp", p = 10)
```

DBSCAN

- **D**ensity-**b**ased **S**patial **C**lustering of **A**pplications with **N**oise
- Label all points as "core points" or "noise points"
  - Core point: has at least m points within radius ε
- Use core points to create clusters
- DBSCAN vs. k-means
  - Noise points are not assigned to any cluster
  - Does not assume spherical shape
- Disadvantages: "curse of dimensionality", the hyperparameters need to be optimized
- Usage – like every other clustering algorithm

```
from sklearn.cluster import DBSCAN
db = DBSCAN(eps = 0.2, min_samples = 5, metric = "euclidean")
```

Example: DBSCAN

- Compare the performance of DBSCAN to the other clustering algorithms
  - Use the previous datasets and results
- Which algorithm performs best on which dataset?
- Clustering comparison in scikit-learn
- Conclusion
  - It's not always obvious which algorithm performs best on a dataset
    - Especially if data comes in many dimensions
  - A successful clustering depends on the algorithm and its hyperparameters
  - We need to choose an appropriate distance metric
  - We need some domain knowledge

Clustering and Classification

- Sometimes, classification tasks can be reduced to clustering tasks
  - Most trivially: just ignore the labels
    - Assumption: The data is easily (e.g., linearly) separable
  - The opposite is also true: we may be able to find a function that assigns a label to each data point
    - This is exactly what clustering does
- We can apply and compare both classification and clustering algorithms, metrics and tools to the same task
  - Even in ensembles
    - Example

Summary

- Unsupervised learning – problem description
- Clustering – problem description, approaches
  - k-means clustering
  - kMeans++
  - Hierarchical clustering
  - DBSCAN
  - Clustering and classification
    - Evaluating clustering / classification performance

Questions?