Geometric Data Analysis

Partitional Clustering

MAT 6480W / STT 6705V

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Fall 2019
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**Challenge:** all classifiers learned so far relied heavily on training with labeled data.

Can we classify without training and extend this approach to work in unsupervised settings?
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Lazy Classifiers

$k$-nearest neighbor classification

Can we classify without training?

Eager & lazy learners in classification

Eager learners train an efficient classification model from labeled data, and then apply this model to new data.

Lazy learners do not train a model at all, but instead infer the class of new data points, as they arrive, from entire labeled training dataset.
Lazy Classifiers

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Lazy learners do not train a model at all, but instead infer the class of new data points, as they arrive, from entire labeled training dataset.

All the classifiers we encountered so far (decision trees, SVM, etc.) are eager learners.
One of the most popular lazy learners is the \( k \) Nearest Neighbors (\( k \)NN) classifier:

**\( k \)NN classifier**

Training: none; use the entire dataset as the classification model.

Classification: given the input

- new point \( y \),
- training data \( X = \{x_1, \ldots, x_N\} \) with labels \( c_1, \ldots, c_N \),
- distance metric \( d(x, y) \), and
- an integer \( 1 \leq k < N \),

find the \( k \) nearest neighbors \( x_{j_1}, \ldots, x_{j_k} \in X \) to \( y \) with respect to the given distance metric, and choose the class that is most common in \( c_{j_1}, \ldots, c_{j_k} \).
The new data point in this case will be classified as ‘+’.
Notice that the classification result may be very sensitive to the exact choice of $k$:

The classification results in these cases will be ‘$-$’ for $k = 1$, uncertain for $k = 2$, and ‘$+$’ for $k = 3$. 
Lazy classifiers

Voronoi diagrams

Consider $k = 1$ and $N$ classes, with one training point from each class. The resulting classifier produces a partition of the space into convex cells, with the training samples as their centroids. In two dimensions such a partition is called a Voronoi diagram.
The $k$-means algorithm aims to find $k$ clusters by using a Voronoi-like partition of the space, where each cluster is contained within a single cell.

**Observation:** given any set of $k$ “centroids”, we can cluster points around them by applying 1-NN classification.

**Question:** how do we get to having a good set of $k$ centroids?

Given a cluster $C = \{x_1, \ldots, x_\ell\}$, we want its centroid $c$ to have a minimal average (squared) distance to other points in the cluster.
Centroid-based classification
\[ k \]-means

Example (Euclidean distance centroid)

We consider points in \( \mathbb{R}^n \) and use the sum of squared errors (a.k.a. scatter)

\[
\text{SSE}(\vec{c}, \vec{x}_1, \ldots, \vec{x}_\ell) = \sum_{i=1}^{\ell} ||\vec{x}_i - \vec{c}||^2 = \sum_{j=1}^{n} \sum_{i=1}^{\ell} (x_{i[j]} - c[j])^2
\]

as a proxy for the average squared distance from the centroid to other points, and compute its minimum by taking:

\[
0 = \frac{\partial \text{SSE}}{\partial c[j]} = \sum_{i=1}^{\ell} \frac{\partial}{\partial c[j]} (x_{i[j]} - c[j])^2 = 2 \sum_{i=1}^{\ell} (x_{i[j]} - c[j])
\]

\[ \Rightarrow \ell c[j] = \sum_{i=1}^{\ell} x_{i[j]} \Rightarrow \vec{c} = \text{mean}\{\vec{x}_1, \ldots, \vec{x}_\ell\} \]
Centroid-based classification

$k$-means

Example (Manhattan distance centroid)

We consider points in $\mathbb{R}^n$ and use the sum of absolute errors

$$\text{SAE}(\vec{c}, \vec{x}_1, \ldots, \vec{x}_\ell) = \sum_{i=1}^{\ell} \|\vec{x}_i - \vec{c}\|_1 = \sum_{j=1}^{n} \sum_{i=1}^{\ell} |x_i[j] - c[j]|$$

as a proxy for the average distance from the centroid to other points, and compute its minimum by taking:

$$0 = \frac{\partial \text{SAE}}{\partial c[j]} = \sum_{i=1}^{\ell} \frac{\partial}{\partial c[j]} |x_i[j] - c[j]| = \sum_{i=1}^{\ell} \text{sign}(x_i[j] - c[j])$$

$$\Rightarrow \#\{x_i[j] \leq c[j]\} = \#\{x_i[j] \geq c[j]\} \Rightarrow \vec{c} = \text{median}\{\vec{x}_1, \ldots, \vec{x}_\ell\}$$
The \( k \)-means algorithm combines the notion of building clusters around centroids and inferring centroids from clusters into one algorithm that iterates these two steps until convergence is reached:

**Initialization:** choose \( k \) random centroids \( c_1, \ldots, c_k \in X \)

**Repeat** the following steps:

- **Assignment:** perform 1-NN classification to (re)assign each \( x \in X \) to one of the cluster centroids
- **Update:** recompute each \( c_j \) to be the centroid of all the points assigned to its cluster

**Until** the centroids/clusters stabilize (i.e., do not change)
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- This algorithm tries to optimize the total SSE/SAE (or equivalent measure) of all the clusters.
- Convergence is guaranteed by SSE/SAE decreasing in each step.
- However, it often finds a local minimum rather than a global one.
Centroid-based classification

$k$-means

Example
Centroid-based classification

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**Example (Bad initialization)**
Since $k$-means performances highly depend on the initialization, it is often run multiple times with random initializations.

Similarly, if the number of clusters is unknown, several values of $k$ can be used in multiple runs.

Finally, the quality of each clustering partition is computed (e.g., with total SSE/SAE) and the best partition is chosen. Notice, however, that the SSE/SAE of clusters will typically decrease when we increase $k$, since the resulting clusters will be smaller.
The “knee method” is a useful SSE-based heuristic for choosing $k$:

Choose $k$ on the “knee” of the curve where its impact on SSE stabilizes (e.g., between 5 and 10 in this plot).
Centroid-based classification
Choosing the number of centroids

Alternatively, one can use the mean silhouette coefficient curve:

Let \( a(x) \) be the mean distance of \( x \) from points in its cluster \( C \):

\[
a(x) = \text{mean}\{\text{dist}(x, y) | y \in C\}
\]

Let \( b(x) \) be the minimal mean distance of \( x \) from other clusters:

\[
b(x) = \min_{\substack{C' \neq C}} \left[\text{mean}\{\text{dist}(x, y) | y \in C'\}\right]
\]

The silhouette coefficient of \( x \) is

\[
s(x) = \frac{b(x) - a(x)}{\max\{a(x), b(x)\}}
\]

In this case \( k \) can be chosen as the peak of the mean silhouette curve (e.g., 10 in this plot).
Other simple steps that may be used to improve & stabilize $k$-means:

**Preprocessing:**
- Normalization / standardization
- Dimensionality reduction
- Outlier elimination

**Postprocessing:**
- Eliminating small clusters
- Splitting “loose” clusters with high SSE/SAE
- Merging close clusters with low combined SSE/SAE

These steps allow a greater initial $k$ to be used, and then reduce the number of clusters in postprocessing.
Extensions and alternatives to $k$-means

$k$-modes

The $k$-means algorithm was formulated with **numerical attributes** in mind, but it can be extended to **nominal data** as well using the $k$-modes algorithm.

Recall that the basic operations in this approach are finding **nearest neighbors** and computing **centroids**, and both rely on **minimizing distances** between centroids and data points in their clusters.

The $k$-modes algorithm uses the **mismatch distance** $d(x, y) = \#\{x[j] \neq y[j]\}$ for both 1-NN and SAE computations. It can be shown that the SAE of a cluster is minimized by **setting $c[j]$ to be the mode** of the $j$-th attribute in the cluster.

The algorithm itself is identical to $k$-means, with the appropriate distance and centroid computations for nominal data.
Extensions and alternatives to $k$-means

Shake & bake

An extension of $k$-means was presented in (David & Averbuch, 2012)\(^1\) as part of the LDF hierarchical clustering. A simplified version is presented here:

**Shake step - random centroid selection**

**Initialize** the set of centroid candidates $V ← X$

**Repeat** the following steps

- Choose a random point $v ∈ V$ as a new centroid
- $V ← V \setminus \{u ∈ V | \text{dist}(u, v) < ε\}$ (for a configurable $ε > 0$)

**Until** $V = ∅$

A partition can then be obtained with $k$-means ($k = \#\text{chosen centroids}$).

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Extensions and alternatives to $k$-means

Shake & bake

Bake step - new clustering distance metric

**Input:** a set of clustering partitions $C_1, \ldots, C_\ell : X \to \mathbb{N}$

For $j = 1, \ldots, \ell$, define

$$D_j(x, y) = \begin{cases} 
0 & x = y \\
0.5 & C_j(x) = C_j(y) \\
1 & C_j(x) \neq C_j(y)
\end{cases}$$

Set $D(x, y) = \ell^{-1} \sum_{j=1}^{\ell} D_j(x, y)$

The final clustering is obtained by using this metric to choose centroids and run $k$-means.
The $k$-means algorithm has two major drawbacks (even for center-based convex clustering):

1. It is sensitive to outliers and noise
2. It requires a good way of choosing centroids

A variation of $k$-means called $k$-medoids aims to alleviate these drawbacks by forcing selected centroids (now called “medoids”) to be actual points observed in the data.

This approach can be realized in several ways (e.g., naively “correct” centroids to nearest data point in the basic $k$-means implementation).
Extensions and alternatives to $k$-means

$k$-medoids & PAM

PAM (Partition Around Medoids) is a popular realization of $k$-medoids that does not require any centroid computation:

**PAM-based $k$-medoids**

**Initialization:** choose $k$ random medoids $c_1, \ldots, c_k \in X$

**Repeat** the following steps:

- **Assignment:** perform 1-NN classification to (re)assign each $x \in X$ to one of the cluster medoids
- **Update:** use random/arbitrary order to scan $X \setminus \{c_1, \ldots, c_k\}$
  
  For each $y \in X \setminus \{c_1, \ldots, c_k\}$ do the following steps:
  - For $i = 1, \ldots, k$, let $\Delta_i = \text{SSE/SAE diff. of setting ‘}c_i \leftarrow y\text{’}$
  - If $\min_i \Delta_i = \Delta_i' < 0$, then set $c_i' \leftarrow y$

**Until** the medoids stabilize (i.e., do not change)

CLARA & CLARANS use sampling to improve the scalability of PAM
Summary

Partitional approaches are distance-based and tend to construct convex-shaped centroid-based clusters.

- Can be regarded as generalization of lazy classifiers to descriptive tasks
- Depend on having appropriate distance notion

The most popular examples of such approaches are $k$-means and its variations.

- Classic versions derived via SSE / SAE
- Sensitive to initialization
- Scalability is a challenge, especially for non-numerical data