Discovering Groups

Summary

Being able to meaningfully cluster data into groups using Clustering or Cluster Analysis is a key part of the process of exploratory and descriptive data mining. Clustering techniques are all a form of unsupervised machine learning. Numerous techniques for clustering exist; in this lecture we'll look at two of the most common and useful: Hierarchical Clustering and K-Means Clustering. We'll also look briefly at a more advanced, but computationally intensive algorithm called Mean Shift Clustering that both produces clusters and finds the *modes* of the data.

Key points

Clustering

- Clustering is an unsupervised machine learning technique, that learns to group data without prior knowledge of what the groups should look like.

Hierarchical Clustering

- Hierarchical Clustering attempts to iteratively break data into a hierarchy of clusters
- Hierarchical Agglomerative Clustering builds a binary tree of clusters from the leaf nodes upwards towards the root
    - Known as a bottom-up approach
    - Requires three things:
        - a set of items to cluster
        - a distance measure to measure how close items are to each other
            - e.g. an Lp distance, a similarity measure converted to a distance (i.e. 1-Pearson or 1-cosine)
            - Doesn't necessarily have to be a distance computed over a vector; some forms of agglomerative clustering allow only need a matrix of distances or similarities computed between all items as input (see below)
        - a linkage criterion which measures dissimilarity of clusters as a function of the pairwise distances of items in the clusters
    - Basic approach:

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■ Initially every item is in a cluster of its own
■ While there is more than one single cluster:
    ■ The closest pair of clusters according to the linkage criterion are merged into a bigger cluster
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        - By recording the merges at each step a binary tree structure linking the clusters can be formed
            - Often a useful way of utilising this is by drawing a diagram known as a dendrogram that shows the structure of the tree
    - Two categories of linkage criterion:

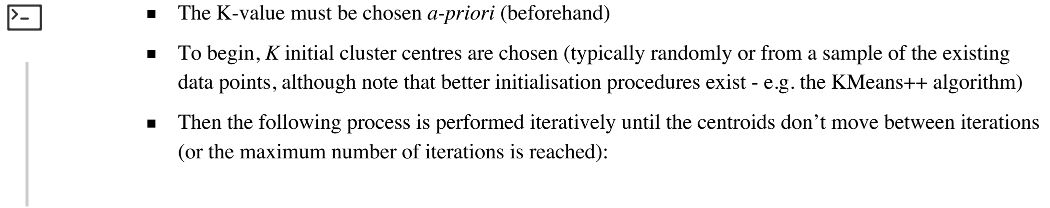
    - Centroid-based linkage functions that measure similarity between clusters based on the distance between their centroids
      - Requires that each item is represented by a numeric feature vector that can be interpreted as a position in space
      - Examples:
        - Weighted Centroid Clustering *(WPGMC - Weighted Pair Group Method with Centroids; often also known as the "median" method)*
          - When two clusters *s* and *t* are combined into a new cluster *u*, the average of centroids *s* and *t* give the new centroid *u*
        - Unweighted Centroid Clustering *(UPGMC - Unweighted Pair Group Method with Centroids)*
          - When two clusters *s* and *t* are combined into a new cluster *u*, the average of the positions of all the items within *s* and *t* give the new centroid *u*
    - Distance-based linkage functions that measure distances between clusters as a function of the distances between items within those clusters.
      - Clustering can be performed purely as a function of a distance matrix in which each element $D_{i,j}$ represents the distance, $d(i,j)$, between items *i* and *j*
      - Commonly used linkage criteria between two sets (clusters) of items *A* and *B* include:
        - Minimum or single-linkage clustering: $\min\{d(a,b) : a \in A, b \in B\}$
          - Drawback: tends to produce long, thin, clusters where the items at each end are far apart
        - Maximum or complete-linkage clustering: $\max\{d(a,b) : a \in A, b \in B\}$
          - Avoids problems of single-linkage clustering; tends to find compact clusters of approximately equal diameter
        - Mean or average linkage clustering (UPGMA - Unweighted Pairwise Group Method with Arithmetic Mean):

$$\frac{1}{|A||B|}\sum_{a \in A}\sum_{b \in B} d(a,b)$$

  - In general, complexity is $O(n^3)$, which can be a problem for large data sets, however there are some $O(n^2)$ variants for the single-linkage and complete-linkage cases
- Divisive clustering algorithms ("top-down" approaches), which start with all the data in the root node and recursively split do exist
  - Not widely used in practice.
    - One major reason is that in general complexity is $O(2^n)$, which is worse than the agglomerative methods.

K-Means Clustering

- The K-Means algorithm (also known as *Lloyds algorithm*) is a simple, but powerful, approach to clustering that attempts to group data in a feature space into K groups or clusters represented by centroids (i.e. the mean point of the class in feature-space).
  - Algorithm:



- The K-value must be chosen *a-priori* (beforehand)
- To begin, *K* initial cluster centres are chosen (typically randomly or from a sample of the existing data points, although note that better initialisation procedures exist - e.g. the KMeans++ algorithm)
- Then the following process is performed iteratively until the centroids don't move between iterations (or the maximum number of iterations is reached):

>   - Each point is assigned to its closest centroid
>   - The centroid is recomputed as the mean of all the points assigned to it. If the centroid has no points assigned it is randomly re-initialised to a new point.
>   - The final clusters are created by assigning all points to their nearest centroid.

    - K-Means always converges, but not necessarily to the most optimal solution

Mean Shift Clustering

- Mean Shift is a standard algorithm to efficiently find the modes of a Probability Density Function (PDF) from a set of samples of that PDF (i.e. the featurevectors representing a set of items).
    - The only variable of the mean shift algorithm is the kernel and the kernel bandwidth of a kernel density estimator.
    - Clustering is an application of the mean shift procedure
        - Automatically chooses the number of clusters!
- The PDF of a continuous random variable is a function that describes the relative likelihood for this random variable to take on a given value
    - The PDF is non-negative everywhere and sums to 1
- In the context of a feature space, the PDF is a function that tells you how likely it is that a featurevector is *drawn* from a specific location in a feature space.
    - A feature vector drawn from part of the space where there are lots of similar items would have a higher probability density than if the drawn feature vector were from a part of the space with very few similar items
        - or in other words, dense parts of the space with more items have a higher probability density
    - Generally speaking, for arbitrary features describing a set of items, the PDF cannot be described empirically
        - Must be estimated using some other method
            - Simple, but crude, way to do this would be to quantise the feature space into bins in order to build a histogram
                - Each bin would contain the count of the number of items with feature vectors falling into that bin divided by the number of total items
                - Major disadvantage of this approach is that it isn't *continuous* and only gives a discrete approximation of the PDF
            - Better way to do this is to use a Kernel Density Estimator (also known as a "Parzen Window")
                - Letting (x_1, x_2, ..., x_n) represent the set of samples (e.g. feature vectors) in a *d*-dimensional space R^d from an unknown density *f*, then:

                  $$f(\mathbf{x}) = \frac{1}{nh^d}\sum_{i=1}^{n} K(\frac{\mathbf{x}-\mathbf{x}_i}{h})$$

                  where $K(\cdot)$ is the kernel (a non-negative function that integrates to one and has mean zero), and $h > 0$ is a smoothing parameter called the kernel bandwidth.
                    - Common choice for the kernel is a multivariate Gaussian with zero mean and unit s.d.
                        - For radially symmetric kernels, it suffices to define the profile of the kernel k(x) satisfying K(x) = $c_{k,d}k(||x||^2)$
                - Intuitively one wants to choose *h* as small as the data will allow
                    - there is always a trade-off between the bias of the estimator and its variance however

- The Mean Shift procedure attempts to find the modes of the density function - that is the points where the gradient is 0: $\nabla f(x)=0$
    - Assuming a radially symmetric kernel, then the gradient is:

$$\nabla f(\mathbf{x}) = \frac{2c_{k,d}}{nh^{d+2}} \sum_{i=1}^{n} (\mathbf{x}-\mathbf{x}_i) g\left(\left\|\frac{\mathbf{x}-\mathbf{x}_i}{h}\right\|^2\right)$$

$$= \frac{2c_{k,d}}{nh^{d+2}} \left[\sum_{i=1}^{n} g\left(\left\|\frac{\mathbf{x}-\mathbf{x}_i}{h}\right\|^2\right)\right] \left[\frac{\sum_{i=1}^{n} \mathbf{x}_i g\left(\left\|\frac{\mathbf{x}-\mathbf{x}_i}{h}\right\|^2\right)}{\sum_{i=1}^{n} g\left(\left\|\frac{\mathbf{x}-\mathbf{x}_i}{h}\right\|^2\right)} - \mathbf{x}\right]$$

      where $g(s)=-k'(s)$.
        - The first term in the above is proportional to the density estimate at x computed with a kernel $G(x)=c_{g,d}g(||x||^2)$, and the second term

$$\mathbf{m}_h(\mathbf{x}) = \frac{\sum_{i=1}^{n} \mathbf{x}_i g\left(\left\|\frac{\mathbf{x}-\mathbf{x}_i}{h}\right\|^2\right)}{\sum_{i=1}^{n} g\left(\left\|\frac{\mathbf{x}-\mathbf{x}_i}{h}\right\|^2\right)} - \mathbf{x}$$

          is the mean shift.
            - The mean shift vector always points toward the direction of the maximum increase in the density.
    - The mean shift procedure, obtained by successive
        - computation of the mean shift vector $m_h(x_t)$,
        - translation of the window $x_{t+1} = x_t + m_h(x_t)$

      is guaranteed to converge to a point where the gradient of density function is zero
- Mean Shift Clustering works as follows:

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- for each feature vector:
    - apply the mean shift procedure until convergence and store the resultant mode
- the set of featurevectors that converge to the same mode define the basin of attraction of that mode; all features
  that converged to the same mode belong to the same cluster
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Further Reading

- Chapter 3 of “Programming Collective Intelligence” gives a good overview of the some of the basic techniques.
- Relevant sections of Chapter 14 of The Elements of Statistical Learning (https://web.stanford.edu/~hastie/ElemStatLearn/printings/ESLII_print10.pdf) provide a good academic introduction
- Wikipedia has reasonable commentary (and good links to the original research) on a number of the topics:
    - https://en.wikipedia.org/wiki/Hierarchical_clustering (https://en.wikipedia.org/wiki/Hierarchical_clustering)
    - https://en.wikipedia.org/wiki/K-means_clustering (https://en.wikipedia.org/wiki/K-means_clustering)
    - https://en.wikipedia.org/wiki/Mean_shift (https://en.wikipedia.org/wiki/Mean_shift)
- k-means++: the advantages of careful seeding (http://ilpubs.stanford.edu:8090/778/1/2006-13.pdf) . Arthur and Vassilvitskii. Proceedings of the eighteenth annual ACM-SIAM symposium on Discrete algorithms. Society for Industrial and Applied Mathematics Philadelphia, PA, USA. pp. 1027–1035. 2007.
- Mean shift: A robust approach toward feature space analysis (http://www.caip.rutgers.edu/riul/research/papers/pdf/mnshft.pdf) . Comaniciu and Meer. IEEE Trans. Pattern Anal. Machine Intell., 24:603–619, 2002.
- Good descriptions of clustering techniques:

- Learning from Data: Concepts, Theory, and Methods (2nd ed.). Cherkassky and Mulier. John Wiley & Sons, Inc., New York, NY, USA.